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NOUVELLE PROTEINE DE FIXATION DU PHOSPHATE, COMPOSITIONS PHARMACEUTIQUES LA CONTENANT ET SES UTILISATIONS

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La présente invention a pour objet une nouvelle protéine, issue du sérum humain, de fixation du phosphate, des compositions pharmaceutiques la contenant ainsi que ses utilisations, notamment dans le cadre du traitement de l'hyperphosphatémie et des maladies cardiovasculaires ou de l'arthrite.

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Le phosphate est une molécule très importante impliquée dans de nombreux mécanismes biologiques. On retrouve notamment le phosphate dans les phospholipides, dans le mécanisme de production d'énergie (ATP, ADP), dans les processus de signalisation cellulaire, dans la composition du matériel génétique dans les os (sous forme de phosphate de calcium).

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L'hyperphosphatémie est une pathologie liée à un excès de phosphate dans l'organisme et provoque notamment une augmentation des risques de maladies cardiovasculaires, en favorisant les processus d'athérosclérose et de calcification des artères (Dorozhkin et Epple, 2002; Amann et al., 2003; Blazheevich et al., 1975). La calcification s'effectuant au niveau des articulations, l'hyperphosphatémie peut aussi provoquer de l'arthrite (pseudo-goutte).

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Les sels de phosphate de calcium produits dans le sérum lors d'une hyperphosphatémie précipitent dans les tissus mous avec calcification ectopique dans différents tissus: vaisseaux (accidents vasculaires cérébraux ou cardiaques), articulations (pseudo-goutte), cristallin, interstitium rénal (néphrocalcinose), souscutanées (prurit), pulmonaires, pancréatiques.

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Ainsi, la moitié des décès chez les personnes souffrant d'insuffisance rénale est due à des maladies cardiovasculaires liées à l'hyperphosphatémie. A cet égard, certains chélateurs du phosphate qui complexent le phosphate dans la lumière intestinale sont actuellement utilisés comme médicament. Cependant, tous ces chélateurs ne sont pas physiologiques. De là découlent certaines complications ou restrictions quant à leur usage.

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Les préparations contenant du magnésium sont limitées par la survenue de troubles digestifs (diarrhée) et sont à proscrire en raison du risque d'hypermagnésémie. De même, la prescription d'hydroxyde d'aluminium, longtemps utilisé du fait de son efficacité, doit être évitée, ou du moins limitée à de très faibles périodes, en raison du

risque d'intoxication aluminique (anémie hypochrome microcytaire, ostéomalacie, myopathie, démence).

La prescription de sels de calcium est le meilleur moyen pour corriger à la fois l'hypocalcémie et l'hyperphosphorémie, permettant d'une part d'augmenter la quantité de calcium absorbée par l'intestin grêle malgré le déficit en calcitriol, et d'autre part de complexer le phosphore dans la lumière intestinale sous forme de phosphate de calcium qui sera éliminé dans les selles. Cependant, l'inconvénient majeur des chélateurs contenant du calcium est d'induire une hypercalcémie, qui, dans certaines séries, a pu être notée chez 20% des malades. Ce risque a conduit à mettre au point d'autres produits capables de limiter l'hyperphosphorémie.

Le médicament actuellement le plus utilisé est le Renagel® (Ramsdell; 1999). Il s'agit d'un polymère cationique, non absorbable capable de chélater le phosphate.

La présente invention a pour but de fournir un nouveau chélateur protéique physiologique se liant au phosphate, ne nécessitant pas l'emploi d'autres ions qui peuvent entraîner des complications et offrant de plus larges perspectives d'utilisation que les chélateurs actuels.

La présente invention concerne une protéine caractérisée en ce qu'elle comprend ou est constituée par :

- la séquence SEQ ID NO: 1,

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- ou toute séquence dérivée de la séquence SEQ ID NO: 1, notamment par substitution, suppression ou addition d'un ou plusieurs acides aminés, sous réserve que ladite séquence dérivée se lie au phosphate,
- ou toute séquence homologue de la séquence SEQ ID NO: 1, ayant de préférence une homologie d'au moins environ 80% avec la séquence SEQ ID NO: 1, sous réserve que ladite séquence homologue se lie au phosphate,
- ou tout fragment d'une des séquences définies ci-dessus, sous réserve que ledit fragment se lie au phosphate, notamment tout fragment étant constitué d'au moins environ 20 acides aminés contigus dans la séquence SEQ ID NO : 1.

La présente invention concerne une protéine telle que définie ci-dessus, caractérisée en ce qu'elle comprend ou est constituée par :

- la séquence SEQ ID NO: 2 ou la séquence SEQ ID NO: 3,
- ou toute séquence dérivée de la séquence SEQ ID NO : 2 ou SEQ ID NO : 3, notamment par substitution, suppression ou addition d'un ou plusieurs acides aminés, sous réserve que ladite séquence dérivée se lie au phosphate,

ou toute séquence homologue de la séquence SEQ ID NO: 2 ou SEQ ID NO: 3, ayant de préférence une homologie d'au moins environ 80% avec la séquence SEQ ID NO: 2 ou SEQ ID NO: 3, sous réserve que ladite séquence homologue se lie au phosphate,

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- ou tout fragment d'une des séquences définies ci-dessus, sous réserve que ledit fragment se lie au phosphate, notamment tout fragment étant constitué d'au moins environ 20 acides aminés contigus dans la séquence SEQ ID NO : 2 ou SEQ ID NO : 3.

La séquence SEQ ID NO: 2 correspond à la protéine humaine de fixation du phosphate. Cette nouvelle protéine a été isolée dans le plasma humain et sa structure tridimensionnelle montre qu'elle appartient à la classe des "phosphate binding protein" (protéines de fixation du phosphate: PBP). Elle est également appelée par la suite HPBP (protéine humaine de fixation du phosphate).

La séquence SEQ ID NO: 3 correspond à une protéine homologue de la protéine de séquence SEQ ID NO: 2, présentant un pourcentage d'identité d'environ 90% avec la séquence SEQ ID NO: 2, et ayant les mêmes propriétés de fixation du phosphate que la séquence SEQ ID NO: 2.

La propriété de fixation du phosphate des séquences de l'invention peut être vérifiée par le test suivant de fixation du phosphate par marquage radioactif :

La protéine est fixée sur une membrane de nitrocellulose (dot blot par aspiration). On laisse incuber la membrane dans un tampon radioactif (³²P (10 mCi/ml, <u>Amersham-Biosciences</u>) 2M; Tris 50 mM; pH 8,0)

La membrane est rapidement rincée 2 × 1 min dans un tampon Tris 50 mM, pH 8,0. En exposant un film photographique avec la membrane (environ 45 min) on peut détecter les zones qui fixent le phosphate radioactif (voir Figure 3 ci-après).

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La présente invention concerne également une séquence nucléotidique codant pour une protéine telle que définie ci-dessus.

La présente invention concerne également un vecteur recombinant, notamment plasmide, cosmide, phage ou ADN de virus, contenant une séquence nucléotidique telle que définie ci-dessus.

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Selon un mode de réalisation avantageux, la présente invention concerne un vecteur recombinant tel que défini ci-dessus, contenant les éléments nécessaires à l'expression dans une cellule hôte des polypeptides codés par la séquence nucléotidique telle que définie ci-dessus, insérée dans ledit vecteur.

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La présente invention concerne également une cellule hôte, choisie notamment parmi les bactéries, les virus, les levures, les champignons, les plantes ou les cellules de mammifères, ladite cellule hôte étant transformée, notamment à l'aide d'un vecteur recombinant tel que défini ci-dessus.

La présente invention concerne également une composition pharmaceutique comprenant à titre de substance active une protéine telle que définie ci-dessus, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, en association avec un véhicule pharmaceutiquement acceptable.

La présente invention concerne également une composition pharmaceutique telle que définie ci-dessus, dans laquelle la protéine de l'invention, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, est en association avec un variant de la protéine paraoxonase, ayant une activité d'hydrolyse du paraoxon.

Parmi les variants de la paraoxonase, on peut citer les variants PON1, PON2, PON3, d'origine humaine ou non, tels que SEQ ID NO : 4 (PON1 humaine ; Hassett et al., 1991), SEQ ID NO : 5 (PON2 humaine ; Primo-Parmo et al., 1996), SEQ ID NO : 6 (PON3 humaine ; Reddy et al., 2001), SEQ ID NO : 7 (PON1 de lapin ; Hassett et al., 1991), SEQ ID NO : 8 (PON1 de rat ; Rodrigo et al., 1997), SEQ ID NO : 9 (PON1 de souris ; Sorenson et al., 1995), SEQ ID NO : 10 (PON2 de souris ; Primo-Parmo et al., 1996) et SEQ ID NO : 11 (PON3 de souris ; Primo-Parmo et al., 1996).

La présente invention concerne également l'utilisation d'une protéine telle que définie ci-dessus, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, pour la préparation d'un médicament destiné à la prévention ou au traitement de maladies liées à une hyperphosphatémie, telles que les maladies cardiovasculaires et l'arthrite (pseudogoutte).

Le terme "hyperphosphatémie" désigne un excès de phosphate dans l'organisme. Plus exactement, l'hyperphosphatémie est définie par une augmentation de la concentration plasmatique de phosphate au dessus de 1,44 mmol/l (45 mg/l), ladite quantité étant obtenue par dosage du phosphate total (le dosage par méthode colorimétrique est effectué après un procédé de minéralisation).

Selon un mode de réalisation avantageux, la protéine de l'invention pourra être administrée sous forme intraveineuse pour pouvoir fixer une quantité maximale de phosphate pendant une longue période, de l'ordre de la semaine. En éliminant ultérieurement la protéine, une grande quantité de phosphate sera ainsi éliminée rapidement. Ceci permet d'espacer et diminuer les temps de dialyse.

La présente invention concerne plus particulièrement l'utilisation d'une protéine telle que définie ci-dessus, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, dans le cadre de la prévention ou du traitement des maladies cardiovasculaires.

La présente invention concerne également l'utilisation d'une protéine selon l'invention, notamment de la protéine représentée par la séquence SEQ ID NO: 2 ou SEQ ID NO: 3, en association avec une protéine telle qu'un variant de la protéine paraoxonase, dans le cadre de la prophylaxie ou du traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques, tels que le soman, le VX, le tabun ou le sarin, ou dans le cadre du traitement de l'athérosclérose.

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La présente invention concerne également un produit de combinaison comprenant au moins une protéine telle que définie ci-dessus, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, et au moins un variant de la protéine paraoxonase, pour une utilisation simultanée, séparée ou étalée dans le temps destiné à la prophylaxie ou au traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques, tels que le soman, le VX, le tabun ou le sarin.

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L'utilisation combinée de la protéine de l'invention, notamment SEQ ID NO : 2, avec un variant de la protéine paraoxonase, permet d'accroître la stabilité de la paraoxonase, notamment dans le cadre de la prophylaxie ou du traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques.

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La présente invention concerne également une méthode de dosage de la protéine telle que définie ci-dessus, caractérisée en ce qu'elle comprend les étapes suivantes :

 des anticorps monoclonaux de lapin dirigé contre différents épitopes de la protéine de l'invention (anti-HPB) sont fixés sur une plaque et le sérum humain à analyser contenant ladite protéine (HPB) est déposé sur la plaque susmentionnée,

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la plaque est rincée et lavée,

- la plaque est rincée et lavée,

on dépose sur la plaque des anticorps anti-anticorps de lapin (anti-IGrabbit-per) marqués avec de la peroxydase durant 30 minutes, afin de former un complexe ternaire entre un anticorps monoclonal de lapin, la protéine selon l'invention et un anticorps anti-anticorps de lapin susmentionnés (anti-HPB – HPB – anti-IGrabbit-per),

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- on fait réagir la peroxydase fixée sur la plaque avec son substrat (kit disponible en commerce, Chemiluminescent Peroxidase Substrate (Sigma)) et la réaction est arrêtée au bout de 30 minutes avec la 3,3',5,5'-tétraméthylbenzidine (TMB, Sigma),

— la densité optique du produit formé à l'étape précédente est mesurée à 450 nm à l'aide d'un spectrophotomètre, et la comparaison de cette mesure avec une courbe étalon permet de déterminer la concentration de la protéine selon l'invention (HPB) présente dans le sérum.

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Ainsi, la méthode de dosage susmentionnée utilise une méthode par immunodosage du type ELISA (Engvall et al., 1971).

D'autres méthodes peuvent être utilisées pour doser la concentration de la protéine de l'invention dans le plasma telles que :

- les méthodes électrophorétiques, ou
- la quantification de son activité.

La présente invention concerne également l'application de la méthode de dosage telle que définie ci-dessus

au diagnostic *in vitro* de maladies liées à une hyperphosphatémie notamment lorsque la quantité de protéine telle que définie ci-dessus, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, dosée selon la méthode telle que définie ci-dessus, est inférieure à la quantité de cette protéine normalement présente dans le sang d'un individu sain, ou

au diagnostic *in vitro* de maladies liées à une hypophosphatémie notamment lorsque la quantité de protéine telle que définie ci-dessus, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, dosée selon la méthode telle que définie ci-dessus, est supérieure à la quantité de cette protéine normalement présente dans le sang d'un individu sain, ou

au diagnostic in vitro d'une prédisposition d'un individu à de telles pathologies.

Le taux de la protéine selon l'invention est un indicateur de prédisposition à un risque de maladie cardiovasculaire. Ainsi, les personnes ayant un taux faible de ladite protéine auront un taux plus important de phosphate libre qui précipitera avec le calcium du plasma pour former des plaques de phosphate de calcium, ce qui est un facteur aggravant notamment les risques de maladies cardiovasculaires ou d'arthrite.

Un taux anormal de cette protéine est aussi le signe d'une pathologie existante. Par exemple une hyperphosphatémie peut déclencher une production accrue de protéine dans le but de limiter le taux de phosphate. Un taux faible peut être lui aussi révélateur d'un dysfonctionnement.

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La présente invention concerne également l'application telle que définie ci-dessus au diagnostic in vitro de maladies liées à une hyperphosphatémie telles que les maladies cardiovasculaires, notamment les maladies cardiovasculaires liées à la formation de

plaques d'athéromes, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement d'une des maladies susmentionnées.

La présente invention concerne également l'application telle que définie ci-dessus au diagnostic in vitro de maladies liées à une hypophosphatémie, ou au diagnostic in vitro d'une prédisposition d'un individu au développement de ces maladies.

Parmi les signes cliniques ou physiologiques caractérisant les maladies liées à une hypophosphatémie, on peut citer :

- une déminéralisation des os,

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- les manifestations musculaires de l'hypophosphatémie qui comportent une myopathie proximale affectant le muscle squelettique et une dysphagie et un iléus affectant les muscles lisses,
 - des carences cardiopulmonaires par le manque d'ATP, et
 - une encéphalopathie métabolique.

LEGENDES DES FIGURES

La Figure 1 représente un gel SDS-PAGE des fractions finales dans le cadre de la purification de la paraoxonase humaine et de la protéine de l'invention SEQ ID NO : 2.

La colonne A correspond au marqueur de poids moléculaire et les colonnes B, C et D à trois purifications différentes issues de différentes poches de plasma humain. Elles contiennent toutes les trois la paraoxonase humaine et la protéine de fixation du phosphate.

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La Figure 2 représente la structure schématique de la protéine de l'invention SEQ ID NO : 2 à laquelle est fixée une molécule de phosphate.

La Figure 3 correspond à un test de fixation du phosphate par la protéine de l'invention SEQ ID NO : 2.

Les colonnes A à F correspondent à différents lots de purification de la protéine de l'invention provenant de différentes poches de plasma humain; la colonne G au lysozyme 1 mg/ml et la colonne H à la β-lacto globuline.

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La Figure 4 représente un gel bidimensionnel d'électrophorèse du mélange de la protéine de l'invention SEQ ID NO : 2 et de la paraoxonase.

La Figure 5 représente les coordonnées moléculaires de la protéine cristallisée de l'invention SEQ ID NO : 2.

PARTIE EXPÉRIMENTALE

Isolation de la protéine

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La protéine SEQ ID NO : 2 est obtenue à partir du plasma humain selon le procédé de Gan et al. (1991) suivant :

La protéine SEQ ID NO: 2 est purifiée à partir de poches de plasma congelé (~200 ml) fournies par l'Etablissement de Transfusion Sanguine de Lyon-Beynost. Le caillot de fibrine, formé par l'ajout de 1 M (1% v/v) de CaCl₂ au plasma est séparé du sérum par filtration. Le sérum est alors mélangé à 400 ml de Gel d'affinité (Cibacron 3GA-Agarose, C-1535, Sigma) équilibré avec un tampon A (Tris/HCl 50 mM, CaCl₂ 1mM, NaCl 4M, pH 8). Dans ces conditions, principalement les HDL ("high density lipoprotein": lipoprotéines de haute densité) sont adsorbées. Après 6 à 8 heures d'incubation, les protéines non adsorbées sur le gel sont éliminées par filtration sur fritté de porosité n°2. Ce lavage s'effectue jusqu'à ce que l'on ne détecte plus de protéine dans l'éluat (absorption UV à 280 nm). Le gel est ensuite équilibré avec un tampon B (Tris/HCl 50 mM, CaCl₂ 1mM, pH 8) puis placé en colonne XK 50/30 (Pharmacia). L'élution est réalisée en rajoutant 1g/l de déoxycholate de sodium et 0,1% de triton X-100 au tampon B. Les fractions montrant une activité arylestérase sont injectées sur 50 ml d'un gel échangeur d'anions (DEAE Sepharose Fast Flow, Pharmacia) disposé en colonne XK 26/70 (Pharmacia) et équilibré avec le tampon B et 0,05% de triton X-100. L'élution se fait par gradient de NaCl. Un premier palier est réalisé à 87,5 mM de NaCl afin d'éliminer l'apo A-I, une protéine liée à la paraoxonase, et la majorité des protéines contaminantes. La paraoxonase humaine (PON1) est environ éluée à la concentration de 140 mM de NaCl. Toutes les fractions conservées montrent une activité paraoxonase et arylestérase, ces activités étant vérifiées selon les tests mentionnés plus loin. Les fractions éluées ne sont pas regroupées. Les gels SDS-PAGE des fractions obtenues montrent des bandes comprises entre 38 kDa et 45 kDa (voir Figure 1). Chaque purification n'apporte pas toujours la même distribution de masse apparente. Cette légère hétérogénéité peut s'expliquer par la présence de 2 chaînes glycosylées sur la PON1.

En plus de la PON1 dans ces lots une autre protéine a été isolée par cristallisation, en substituant le triton par le C12-maltoside et en utilisant le sulfate d'ammonium comme agent précipitant. Les cristaux obtenus sont ceux d'une protéine inconnue caractérisée par radiocristallographie et correspondant à la séquence SEQ ID NO : 2 de

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l'invention. La cristallisation est actuellement le seul procédé existant pour purifier cette protéine.

L'activité paraoxonase est mesurée dans un tampon Glycine 50 mM/NaOH, CaCl₂ 1 mM, en présence de 1 M NaCl, pH 10,5 et est déterminée au moyen d'un spectrophotomètre à double faisceau (Shimadzu UV 160A) thermostaté à 25°C. La vitesse d'hydrolyse est déterminée d'après la variation d'absorbance à 412 nm, correspondant à la formation de p-nitrophénol libéré par l'hydrolyse de paraoxon, en fonction du temps, $\varepsilon = 18290 \, \text{M}^{-1} \text{cm}^{-1}$ (Smolen, 1991).

L'activité arylestérase est mesurée dans un tampon tris 50mM/HCl, $\text{CaCl}_2\ 1\text{mM}$, pH 8 et est déterminée au moyen d'un spectrophotomètre à double faisceau (Shimadzu UV 160A) thermostaté à 25°C . La vitesse d'hydrolyse est déterminée d'après la variation d'absorbance à 270 nm, correspondant à la formation de phénol libéré par l'hydrolyse de phényl acétate, en fonction du temps, $\varepsilon = 1310 \, \text{M}^{-1} \text{cm}^{-1}$ (Smolen, 1991).

Structure

La structure de la protéine cristallisée SEQ ID NO: 2 a été obtenue par cristallographie des rayons X. La structure à 1,9 Å de résolution a été obtenue par la méthode SIRAS (Single Isomorphous Replacement and Anomalous Scattering)(Figure 2).

Les données de diffraction des rayons X ont été collectées sur la ligne BM30 de l'ESRF (Grenoble).

Un dérivé de sel d'atome lourd a été obtenu en trempant un cristal dans une solution contenant des sels d'uranium.

Les images ont été intégrées, mises à l'échelle et combinées avec les programmes XDS2000 (Kabsch, 1993) et la suite CCP4 (COLLABORATIVE COMPUTATIONAL PROJECT, NUMBER 4. 1994. "The CCP4 Suite: Programs for Protein Crystallography". Acta Cryst. D50, 760-763).

Les programmes CNS (BRUNGER, 1998) et SnB (Weeks, 1999) ont été utilisés pour localiser les atomes d'uranium. Le programme SHARP (Copyright © 2001-2002 the Buster Development Group) a été utilisé pour obtenir les phases par la technique SIRAS.

372 acides aminés ont été construits automatiquement dans la carte de densité électronique par le programme ARP/wARP (Perrakis, 1997). Ce premier modèle a ensuite été affiné par le programme CNS.

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En raison de la très bonne qualité des cartes de densité électronique, la séquence primaire de la protéine a pu être assignée avec 80% de fiabilité. Une molécule de phosphate a aussi pu être localisée.

La structure obtenue ne correspond pas du tout à la paraoxonase humaine. Le séquençage obtenu en identifiant les acides aminés à partir de la densité électronique indique que ni cette protéine humaine ni son gène n'ont été décrits auparavant. Il s'agit donc d'une nouvelle protéine.

La structure de la protéine de l'invention montre une très forte homologie avec la protéine de fixation du phosphate ("phosphate binding") d'*Escherichia coli*. Cette protéine chez cette bactérie sert à transporter le phosphate à travers le périplasme. On la retrouve chez beaucoup de procaryotes mais chez aucun eucaryote.

La densité électronique a aussi montré qu'une molécule de phosphate était fixée à la nouvelle protéine de l'invention, de la même façon que dans celle d'Escherichia coli.

Ainsi, on peut conclure que la protéine de l'invention caractérisée à partir du plasma humain présente une très forte homologie avec la protéine bactérienne et qu'elle est capable de fixer le phosphate et de le transporter.

Séquençage

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Digestion dans le gel

Le mélange paraoxonase-HPBP a été séparé par gel électrophorétique avec SDS-PAGE (sans chauffage). Plusieurs bandes correspondant à HPBP aux alentour de 70 kDa ont été découpées.

La digestion de la protéine contenue dans ces bandes a été effectuée grâce au système automatique de digestion, MassPrep Sation (Waters Manchester, G.B.). Les bandes de gel ont été lavées deux fois avec 50 μl d'une solution à 25 mM de carbonate d'ammonium hydrogéné (NH₄HCO₃) et 50 μl d'acétonitrile. Les cystéines ont été réduites avec 50 μl d'une solution à 10mM de dithiothréitol à 57°C et acylé avec 50 μl de iodocacétamide à 55 mM. Après déshydratation avec l'acétonitrile, la protéine a été digérée enzymatiquement avec 10 μl de trypsine porcine modifiée à 12,5 ng/μl (Promega, Madisson, WI, U.S.A) ou bien avec lys-C de Lysobacter enzymogenes (Roche Applied Science, Penzberg, Germany) dans 25 mM de NH₄HCO₃. La digestion s'est opérée une nuit complète à température ambiante. Les peptides clivés ont été extraits avec une solution à 60% d'acétonitrile et 5% d'acide formique.

Analyse par spectrométrie de masse

MALDI-MS et MALDI-MS/MS

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Les mesures de masse par MALDI-TOF on été effectuées sur un UltraflexTM TOF/TOF (Bruker, Daltonik GmbH, Brème, Allemagne). Cet instrument a été utilisé avec un potentiel d'accélération maximum de 25 KV dans le mode reflectron. L'échantillon a été préparé avec la préparation standard de la goutte asséchée sur la cible en acier inoxydable en utilisant comme matrice l'acide α-cyano-4-hydroxycinnamique.

La calibration externe du spectre MALDI-MS a été effectuée en utilisant seulement les pics des charges mono isotopiques d'une solution connue de peptides (bradykinine 1-7 (m/z=757,400), angiotensine humaine II (m/z=1046,542), angiotensine humaine I (m/z=1296,685), substance P (m/z=1347,735), bombesine (m/z=1619,822), renine (m/z=1758,933), ACTH 1-17 (m/z=2093,087) et ACTH 18-39 (m/z=2465,199)). Les masses des peptides mono isotopiques ont été automatiquement annotées grâce au programme Flexanalysis 2.0.

Les spectres MS/MS ont été obtenus par l'analyse des ions métastables obtenus par "Laser-Induced Decomposition" (LID) d'un précurseur ioniques sectionné, sans collision additionnelle en phase gazeuse. Le précurseur ionique a été accéléré à 8kV et a été sélectionné grâce à une trappe à ions à sélection temporelle. Les fragments ont été par la suite accélérés à 19 kV dans la cellule LIFT et leurs masses mesurées après leurs passages sur le réflecteur ionique.

Le séquençage de novo de chacun de ces spectres MS/MS a été effectué avec le programme Full DeNovo Sequencing program (Biotools, Bruker Daltonik GmbH, Brème, Allemagne).

NanoLC-MS/MS

L'analyse NanoLC-MS/MS a été effectuée en utilisant un CapLC (Waters, Manchester, G.B.) couplé à un spectromètre de masse "temps de vol" accéléré par un quadripôle hybride orthogonal Q-TOF II ((Micromass, Manchester, G.B.). La séparation par chromatographie en phase inverse à été effectuée avec des capillaires (Pepmap C18, 75 µm i.d., 15 cm de long, LC Packings) sous un flux à 200 nL/min, maintenu constant grâce à une pré-colonne de partage. La calibration a été effectuée en utilisant 2pmol/µl de GFP.

L'acquisition des données de masse a été pilotée par le programme MassLynx (Micromass, Manchester, G.B.) qui bascule automatiquement entre le mode MS et le mode MS/MS.

Les spectres MS/MS générés ont été individuellement séquencés de novo afin d'obtenir la séquence partielle ou complète. Ces interprétations ont été réalisées en utilisant le programme PepSeq (MassLynx, Micromass) et le programme PEAKS Studio (Bioinformatics Solutions, Waterloo, Canada) qui sont capables de traiter complètement un fichier pkl avec un séquençage de novo automatique sur chaque spectre MS/MS.

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Fixation du phosphate

La fixation du phosphate par la protéine de l'invention SEQ ID NO : 2 a été mise en évidence selon le test suivant :

On dépose 200 µl de la protéine de l'invention SEQ ID NO : 2 (colonnes A-F de la Figure 3), ou du lysozyme 1 mg/ml (colonne G) ou de la βlacto-globuline sur nitrocellulose (dot blot par aspiration).

L'ensemble est incubé pendant 2 h 30 dans un mélange comprenant : tris 50 mM; pH 8,0; ³²P (10 mCi/ml) 2 mM.

On effectue ensuite un rinçage 2 fois pendant 1 minute avec du tris 50 mM à pH 8,0, puis on expose l'ensemble à température ambiante pendant 45 minutes.

On constate alors (voir Figure 3) que la protéine de l'invention a fixé le phosphate radioactif (colonnes A à F), alors que les témoins tests ne l'ont pas fixée (colonnes G et H).

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Rôle et utilisation de la protéine SEO ID NO: 2

Pour doser la concentration de cette protéine dans le plasma les méthodes utilisables sont :

- les methodes électrophorétiques,
- la purification de la protéine,
- la quantification de son activité,
- l'immunodosage de la protéine en utilisant des anticorps polyclonaux/monoclonaux dirigé contre la protéine.

Association avec la paraoxonase

Electrophorèse bidimensionnelle

Les protéines purifiées (40 µg) comme dans le protocole décrit précédemment sont mélangées à 100 µL d'une solution contenant 9,8 M d'urée, 4% (v/v) triton X100, 2 mM tributyl phosphine, 0,2 % (v/v) d'ampholine 3-10 (Bio-Lytes 3 -10; Bio-Rad), et 0,001% (m/v) de bleu de bromophénol. Des bandelettes (IPG-Strips; Bio-Rad) de gel de polyacrylamide (T: 4 %; C: 3 %) prêtes à l'emploi sont utilisées. Des ampholines ont été fixées de manière covalente au polyacrylamide de sorte d'avoir un gradient linéaire de pH pré-établi. Le gradient de pH utilisé est entre 3,0 et 10,0.

1. Isoélectrofocation (IEF)

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Les bandelettes sont placées en contact avec les échantillons protéiques dans l'appareil Protean IEF Cell (Bio-Rad) et réhydratées activement (50 V constant) pendant 15 heures à 20°C. L'isoélectrofocalisation est ensuite réalisée en 3 étapes à 20°C. Premièrement un faible voltage de 250 V est appliqué pendant 15 minutes ; deuxièmement, une montée en gradient de 250 à 4000 V (ampérage limité par bandelette à 50 μA) est programmée sur 2 h. Troisièmement, le voltage est maintenu constant à 4000 V pendant 4 heures. Après migration, les bandelettes sont conservées à -20 °C.

D'après le protocole de purification précédent, la protéine HPBP de l'invention est co-purifiée avec la paraoxonase humaine (PON)(Fokine et al., 2003). En faisant un gel bidimensionnel avec le protocole ci-dessus, 2 spots ont été identifiés par séquençage N-terminal comme étant respectivement la protéine de l'invention HPBP et la paraoxonase humaine (voir Figure 4). Les deux protéines ont approximativement la même masse moléculaire (environ 40 kDa) et des points isoélectriques distincts, 6.9-8.5 pour HPBP et 4-5 pour la PON1. En tenant compte du fait qu'il a fallu utiliser des conditions drastiques pour réussir à séparer sur gel les 2 protéines (9M d'urée et 4% de triton)et que les 2 protéines qui ont des points isoélectriques très différents restent co-purifiées après le passage dans une colonne échangeuse d'anion (DEAE sepharose), on conclut qu'elles sont associées en formant un complexe.

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REVENDICATIONS

- 1. Protéine caractérisée en ce qu'elle comprend ou est constituée par :
- la séquence SEQ ID NO: 1,
- ou toute séquence dérivée de la séquence SEQ ID NO: 1, notamment par substitution, suppression ou addition d'un ou plusieurs acides aminés, sous réserve que ladite séquence dérivée se lie au phosphate,
- ou toute séquence homologue de la séquence SEQ ID NO: 1, ayant de préférence une homologie d'au moins environ 80% avec la séquence SEQ ID NO: 1, sous réserve que ladite séquence homologue se lie au phosphate,
- ou tout fragment d'une des séquences définies ci-dessus, sous réserve que ledit fragment se lie au phosphate, notamment tout fragment étant constitué d'au moins environ 20 acides aminés contigus dans la séquence SEQ ID NO : 1.
- 2. Protéine selon la revendication 1, caractérisée en ce qu'elle comprend ou est constituée par :
 - la séquence SEQ ID NO : 2 ou SEQ ID NO : 3,
- ou toute séquence dérivée de la séquence SEQ ID NO : 2 ou SEQ ID NO : 3, notamment par substitution, suppression ou addition d'un ou plusieurs acides aminés, sous réserve que ladite séquence dérivée se lie au phosphate,
- ou toute séquence homologue de la séquence SEQ ID NO: 2 ou SEQ ID NO: 3, ayant de préférence une homologie d'au moins environ 80% avec la séquence SEQ ID NO: 2 ou SEQ ID NO: 3, sous réserve que ladite séquence homologue se lie au phosphate,
- ou tout fragment d'une des séquences définies ci-dessus, sous réserve que ledit fragment se lie au phosphate, notamment tout fragment étant constitué d'au moins environ 20 acides aminés contigus dans la séquence SEQ ID NO : 2 ou SEQ ID NO : 3.
- 3. Séquence nucléotidique codant pour une protéine telle que définie dans la revendication 1 ou 2.
- 4. Vecteur recombinant, notamment plasmide, cosmide, phage ou ADN de virus, contenant une séquence nucléotidique selon la revendication 3.

5. Vecteur recombinant selon la revendication 4, contenant les éléments nécessaires à l'expression dans une cellule hôte des polypeptides codés par une séquence nucléotidique selon la revendication 3, insérés dans ledit vecteur.

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6. Cellule hôte, choisie notamment parmi les bactéries, les levures, les cellules de champignons, les cellules de plantes ou les cellules de mammifères, ladite cellule hôte étant transformée à l'aide d'un vecteur recombinant selon l'une des revendications 4 ou 5.

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7. Composition pharmaceutique comprenant à titre de substance active une protéine selon la revendication 1 ou 2, en association avec un véhicule pharmaceutiquement acceptable.

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8. Composition pharmaceutique selon la revendication 7, comprenant à titre de substance active une protéine représentée par la séquence SEQ ID NO : 2 ou SEQ ID NO : 3.

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9. Composition pharmaceutique selon la revendication 8, dans laquelle la protéine telle que définie dans la revendication 1 ou 2, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, est en association avec un variant de la protéine paraoxonase, notamment SEQ ID NO: 4, SEQ ID NO: 5, SEQ ID NO: 6, SEQ ID NO: 7, SEQ ID NO: 8, SEQ ID NO: 9, SEQ ID NO: 10 ou SEQ ID NO: 11.

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10. Utilisation d'une protéine selon la revendication 1 ou 2, notamment de la protéine représentée par la séquence SEQ ID NO: 2 ou SEQ ID NO: 3, pour la préparation d'un médicament destiné à la prévention ou au traitement de l'arthrite ou de maladies liées à une hyperphosphatémie, telles que les maladies cardiovasculaires, ou, en association avec un variant de la protéine paraoxonase, notamment SEQ ID NO: 4, SEQ ID NO: 5, SEQ ID NO: 6, SEQ ID NO: 7, SEQ ID NO: 8, SEQ ID NO: 9, SEQ ID NO: 10 ou SEQ ID NO: 11, dans le cadre de la prophylaxie ou du traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques tels que le soman, le VX, le sarin ou le tabun, ou dans le cadre du traitement de l'athérosclérose.

- 11. Produit de combinaison comprenant au moins une protéine selon la revendication 1 ou 2, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, et au moins un variant de la protéine paraoxonase, notamment SEQ ID NO: 4, SEQ ID NO: 5, SEQ ID NO: 6, SEQ ID NO: 7, SEQ ID NO: 8, SEQ ID NO: 9, SEQ ID NO: 10 ou SEQ ID NO: 11, pour une utilisation simultanée, séparée ou étalée dans le temps destiné à la prophylaxie ou au traitement des intoxications provoquées par des insecticides ou des agents neurotoxiques tels que le soman, le VX, le sarin ou le tabun.
- 12. Méthode de dosage de la protéine selon la revendication 1 ou 2, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, caractérisée en ce qu'elle comprend les étapes suivantes:
- des anticorps monoclonaux de lapin dirigé contre différents épitopes de la protéine selon la revendication 1 ou 2, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, sont fixés sur une plaque et le sérum humain à analyser contenant ladite protéine est déposé sur la plaque susmentionnée,
 - la plaque est rincée et lavée,

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- on dépose sur ladite plaque des anticorps anti-anticorps de lapin marqués avec de la peroxydase durant 30 minutes, afin de former un complexe ternaire entre un anticorps monoclonal de lapin, ladite protéine et un anticorps anti-anticorps de lapin susmentionnés,
 - la plaque est rincée et lavée,
- on fait réagir la peroxydase fixée sur la plaque avec son substrat et la réaction est arrêtée au bout de 30 minutes avec la 3,3',5,5'-tétraméthylbenzidine,
- la densité optique du produit formé à l'étape précédente est mesurée à 450 nm à l'aide d'un spectrophotomètre, et la comparaison de cette mesure avec une courbe étalon permet de déterminer la concentration de la protéine selon la revendication 1 ou 2, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, présente dans le sérum.

13. Application de la méthode de dosage selon la revendication 12

au diagnostic *in vitro* de maladies liées à une hyperphosphatémie notamment lorsque la quantité de protéine selon la revendication 1 ou 2, notamment SEQ ID NO : 2 ou SEQ ID NO : 3, dosée selon la méthode de la revendication 12, est inférieure à la quantité de cette protéine normalement présente dans le sang d'un individu sain, ou

au diagnostic *in vitro* de maladies liées à une hypophosphatémie notamment lorsque la quantité de protéine selon la revendication 1 ou 2, notamment SEQ ID NO: 2 ou SEQ ID NO: 3, dosée selon la méthode de la revendication 12, est supérieure à la quantité de cette protéine normalement présente dans le sang d'un individu sain, ou au diagnostic *in vitro* d'une prédisposition d'un individu à de telles pathologies.

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14. Application selon la revendication 13 au diagnostic *in vitro* de maladies liées à une hyperphosphatémie telles que les maladies cardiovasculaires, notamment les maladies cardiovasculaires liées à la formation de plaques d'athéromes, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement d'une des maladies susmentionnées.

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15. Application selon la revendication 14 au diagnostic *in vitro* de maladies liées à une hypophosphatémie, ou au diagnostic *in vitro* d'une prédisposition d'un individu au développement de ces maladies.

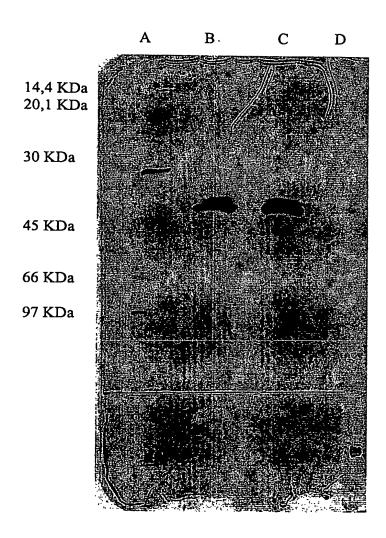


FIGURE 1

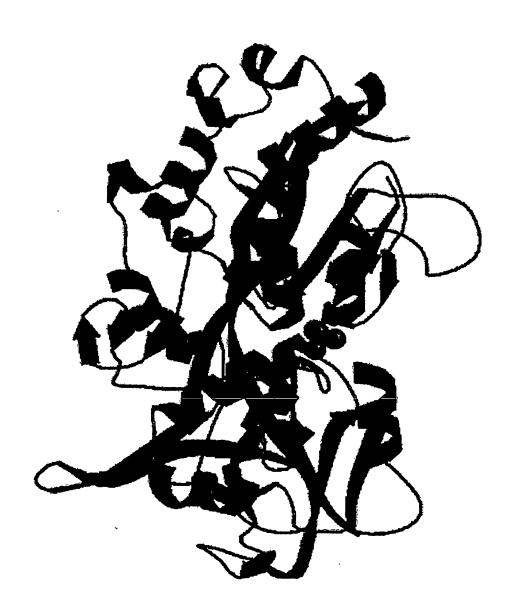


FIGURE 2

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A B C D E F G H

FIGURE 3

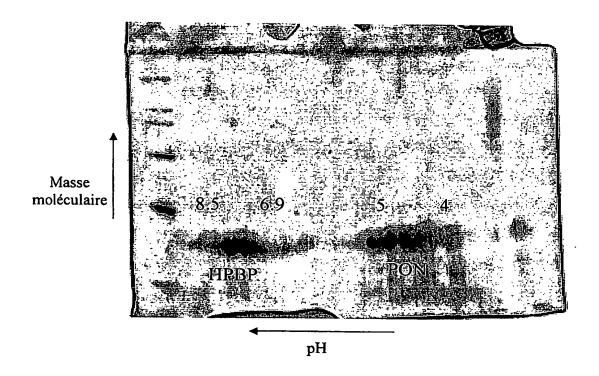


FIGURE 4

ATOM	1	CB	SER .	A 1	24.666	45.653	14.370	1.00 26.15	A
ATOM	2	OG	SER	A 1	25.258	46.028	13.130	1.00 38.82	A
ATOM	3	C	SER		22.519	45.324	15.622	1.00 20.30	A
ATOM	4	0	SER A		21.889	46.093	16.367	1.00 18.83	Ą
MOTA ATOM	5 6	N CA	SER A	A 1 A 1	22.817 23.146	47.273 45.831	14.074 14.317	1.00 22.37 1.00 22.87	A A
ATOM	7	N	ILE 2		22.676	44.027	15.878	1.00 14.00	Ā
ATOM '	8	CA	ILE A	A 2	22.149	43.401	17.092	1.00 13.36	A
ATOM	9	CB	ILE A		21.747	41.923	16.828	1.00 14.04	A
ATOM ATOM	10 11	CG2 CG1	ILE A		21.536	41.191	18.155 15.988	1.00 9.05	A
ATOM	12	CD1			20.458 20.173	41.872 40.501	15.357	1.00 13.38 1.00 14.27	A A
ATOM	13	C	ILE 2	A 2	23.303	43.459	18.083	1.00 12.32	A
ATOM	14	0	ILE A		24.376	42.890	17.847	1.00 14.26	A
ATOM ATOM	15 16	N CA	ASP ASP		23.075 24.134	44.122	19.205	1.00 13.19	A
ATOM	17	CB	ASP A		24.134	44.331 45.830	20.193 20.578	1.00 11.15 1.00 12.52	A A
MOTA	18	CG	ASP A	A 3	24.268	46.744	19.351	1.00 11.70	A
ATOM	19	OD1			25.289	46.618	18.642	1.00 11.97	A
ATOM ATOM	20 21,	OD2 C	ASP A	_	23.356 23.981	47.569 43.508	19.094 21.456	1.00 13.82 1.00 11.88	A A
ATOM	22	ŏ	ASP A		22.947	43.577	22.116	1.00 11.88	A
MOTA	23	N	GLY A	A 4	25.022	42.763	21.800	1.00 9.46	A
ATOM	24	CA	GLY A		24.973	41.947	23.007	1.00 10.97	A
MOTA MOTA	25 26	CO	GLY A		26.303 27.314	41.966 42.413	23.740 23.200	1.00 8.48 1.00 9.87	A A
ATOM	27	Ň	GLY A		26.296	41.496	24.987	1.00 11.77	Â
MOTA	28	CA	GLY A	A 5	27.511	41.489	25.785	1.00 4.85	A
ATOM ATOM	29	C	GLY A		27.163	41.000	27.186	1.00 8.06	A
ATOM	30 31	O N	GLY A		26.009 28.144	40.610 41.021	27.447 28.089	1.00 9.13 1.00 9.80	A A
ATOM	32	CA	GLY A		27.898	40.589	29.458	1.00 9.86	A
MOTA	33	C	GLY A		28.970	39.679	30.014	1.00 7.11	Α
ATOM ATOM	34 35	O N	GLY ALA		30.150	40.030	30.000	1.00 8.89	A
ATOM	36	CA	ALA A		28.567 29.509	38.518 37.540	30.525 31.079	1.00 9.08 1.00 8.69	A A
ATOM	37	CB	ALA A	A 7	28.814	36.168	31.195	1.00 7.94	Ä
ATOM	38	C	ALA A		30.811	37.363	30.277	1.00 9.69	A
ATOM ATOM	39 40	O N	ALA A		30.781 31.941	37.212 37.367	29.050 30.981	1.00 7.30 1.00 7.56	A A
ATOM	41	CA	THR A		33.236	37.135	30.338	1.00 7.30	A
MOTA	42	CB	THR A	8 4	34.402	37.865	31.065	1.00 8.00	A·
ATOM ATOM	43	OG1 CG2	THR A		34.532	37.344	32.402	1.00 9.83	. A
ATOM	44 45	CGZ	THR A		34.123 33.542	39.388 35.624	31.139 30.340	1.00 10.68 1.00 5.67	A A
ATOM	46	ŏ	THR A	_	34.355	35.168	29.552	1.00 8.00	A
ATOM	47	N	LEU A		32.885	34.842	31.195	1.00 6.65	A
MOTA MOTA	48 49	CA CB	LEU A		33.190 32.275	33.389 32.649	31.224 32.238	1.00 9.98 1.00 10.55	A
ATOM	50	CG	LEU A		32.400	31.109	32.271	1.00 10.55	A A
ATOM	51	CD1	LEU A	A 9	32.200	30.566	33.699	1.00 10.77	A
ATOM	52	CD2	LEU A		31.356	30.503	31.300	1.00 6.94	A
ATOM ATOM	53 54	C	LEU A		33.103 33.985	32.755 31.970	29.817 29.421	1.00 10.91 1.00 9.67	A A
ATOM	55	Ñ	PRO A		32.051	33.088	29.040	1.00 6.59	Ä
ATOM	56	CD	PRO A		30.763	33.664	29.485	1.00 8.09	A
ATOM ATOM	57 58	CA CB	PRO P		31.915 30.428	32.521 32.218	27.686 27.611	1.00 7.68 1.00 11.73	A
ATOM	59	CG	PRO A		29.845	33.467	28.251	1.00 11.73	A A
ATOM	60	С	PRO A	10	32.317	33.504	26.579	1.00 8.72	A
ATOM	61	o.	PRO A		32.040	33.263	25.396	1.00 9.01	A
ATOM ATOM	62 63	N CA	GLU A		33.003 33.325	34.589 35.565	26.928 25.896	1.00 5.35 1.00 8.04	A A
ATOM	64	CB	GLU A		33.978	36.829	26.493	1.00 12.60	A
ATOM	65	CG	GLU A	11	35.380	36.672	27.001	1.00 21.32	A
ATOM	66	CD	GLU A		35.994	38.013	27.391	1.00 26.61	A
ATOM ATOM	67 68	OE1 OE2	GLU F		35.264 37.203	38.873 38.202	27.920 27.176	1.00 30.93 1.00 31.32	A A
ATOM	69	C	GLU A		34.143	35.066	24.709	1.00 10.00	A
ATOM	70	0	GLU A	11	33.866	35.464	23.563	1.00 8.68	Α
ATOM ATOM	71 72	N CA	LYS A		35.134 35.935	34.215 33.678	24.957	1.00 8.65 1.00 10.43	A N
ATOM	73	CB	LYS A		37.081	32.840	23.850 24.374	1.00 10.43	A A
MOTA	74	CG	LYS A	12	38.151	33.646	25.090	1.00 9.26	A
ATOM	75	CD	LYS A		39.117	32.622	25.673	1.00 17.64	Α

ATOM ATOM	76 77	CE NZ	LYS A		40.293	33.277	26.307	1.00 24.93	A
ATOM	78	C	LYS A		41.298 35.079	32.237 32.830	26.600 22.934	1.00 25.96 1.00 11.17	A
ATOM	79	0	LYS A	12	35.339	32.726	21.736	1.00 11.17	A A
ATOM ATOM	80 81	N CA	LEU A		34.071	32.176	23.498	1.00 7.67	A
ATOM	82	CB	LEU A		33.189 32.230	31.383 30.549	22.669 23.534	1.00 10.04 1.00 8.86	A A
ATOM	83	CG	LEU A		31.082	29.888	22.769	1.00 8.97	A
ATOM ATOM	84 85	CD1 CD2			31.649 30.101	28.807	21.805	1.00 12.12	A
ATOM	86	С	LEU A	. 13	32.371	29.268 32.292	23.753 21.750	1.00 12.69 1.00 9.01	A A
ATOM ATOM	87 88	N O	LEU A		32.293	32.064	20.536	1.00 10.60	A
ATOM	89	CA	TYR A		31.761 30.920	33.329 34.195	22.305 21.482	1.00 10.47 1.00 9.03	A A
ATOM ATOM	90	CB	TYR A		30.029	35.087	22.352	1.00 8.38	A
ATOM	91 92	CG CD1	TYR A		29.091 28.499	34.293 33.109	23.253 22.806	1.00 11.48 1.00 12.01	A
MOTA	93	CE1	TYR A	14	27.671	32.341	23.642	1.00 12.01 1.00 10.45	A A
ATOM ATOM	94 95	CD2 CE2	TYR A		28.824 27.998	34.706	24.564	1.00 10.30	Α
ATOM	96	cz	TYR A	14	27.430	33.948 32.766	25.403 24.933	1.00 10.35 1.00 8.21	A A
ATOM ATOM	97 98	С ОН	TYR A		26.628	32.014	25.757	1.00 8.65	A
MOTA	99	ŏ	TYR A		31.715 31.142	35.036 35.538	20.489 19.515	1.00 9.67 1.00 8.36	A A
ATOM ATOM	100 101	N	LEU A		33.021	35.184	20.738	1.00 8.53	Ä
ATOM	102	CA CB	LEU A		33.904° 35.087	35.936 36.564	19.838 20.601	1.00 9.45 1.00 8.09	A A
ATOM	103	CG	LEU A	15	34.742	37.802	21.433	1.00 14.85	A
ATOM ATOM	104 105	CD1 CD2	LEU A	15 15	35.932 34.364	38.141 38.990	22.306 20.510	1.00 16.07	A
ATOM	106	С	LEU A	15	34.467	35.018	18.756	1.00 12.61 1.00 16.00	A A
ATOM ATOM	107 108	O N	LEU A	15 16	35.174 34.178	35.466 33.729	17.859	1.00 16.13	A
ATOM	109	CA	THR A	16	34.681	32.791	18.848 17.853	1.00 11.70 1.00 11.09	A A
ATOM ATOM	110 111	CB OG1	THR A	16	34.523	31.334	18.371	1.00 11.33	A
ATOM	112	CG2	THR A	16 16	35.406 34.848	31.142 30.314	19.484 17.291	1.00 13.08 1.00 11.23	A A
ATOM	113	C	THR A	16	33.906	32.997	16.549	1.00 12.10	Ä
ATOM ATOM	114 115	O N	THR A	16 17	32.671 34.620	32.996 33.158	16.540 15.420	1.00 12.20 1.00 14.18	A
ATOM	116	CD	PRO A	17	36.085	33.162	15.251	1.00 14.83	A A
ATOM ATOM	117 118	CA CB	PRO A	17 17	33.933 35.068	33.367 33.292	14.137 13.113	1.00 17.90 1.00 20.97	A
ATOM	119	CG	PRO A	17	36.251	33.842	13.890	1.00 20.97	A A
ATOM ATOM	120 121	C O	PRO A	17 17	32.830 33.027	32.341 31.143	13.854	1.00 14.42	A
MOTA	122	N	ASP A	18	31.673	32.836	14.066 13.414	1.00 14.18 1.00 15.17	A A
ATOM ATOM	123 124	CA CB	ASP A	18 18	30.515 30.932	32.020 30.829	13.058	1.00 19.19	A
ATOM	125	CG	ASP A	18	31.649	31.260	12.169 10.885	1.00 23.04 1.00 30.30	A A
ATOM ATOM	126	OD1		18	31.214	32.238	10.239	1.00 30.86	A
ATOM	127 128	C	ASP A	18 18	32.645 29.657	30.599 31.479	10.511 14.212	1.00 39.65 1.00 13.08	A A
ATOM	129	0	ASP A	18	28.651	30.833	13.958	1.00 13.28	A
ATOM	130	N CA	VAL A	19 19	30.041 29.199	31.709 31.221	15.466 16.570	1.00 13.07 1.00 8.94	A A
ATOM	132	CB	VAL A	19	29.976	31.225	17.911	1.00 9.65	Ä
ATOM ATOM	133 134	CG1 CG2		19 19	29.014 30.930	31.123 30.026	19.098 17.923	1.00 11.73 1.00 11.99	A A
MOTA	135	Ç	VAL A	19	27.971	32.126	16.613	1.00 11.81	Â
ATOM ATOM	136 137	O N	VAL A LEU A	19 20	26.829 28.198	31.655	16.707	1.00 11.21	A
MOTA	138	CA	LEU A	20	27.077	33.434 34.363	16.567 16.486	1.00 10.93 1.00 8.58	A A
ATOM	139	CB	LEU A	20	27.439	35.730	17.084	1.00 13.44	A
ATOM ATOM	140 141	CG CD1	LEU A	20 20	27.677 27.863	35.767 37.222	18.601 19.084	1.00 14.24 1.00 13.26	A A
ATOM	142	CD2	LEU A	20	26.480	35.130	19.315	1.00 11.94	A
ATOM ATOM	143 144	C O	LEU A	20 20	26.857 27.836	34.470 34.550	14.969 14.196	1.00 15.21 1.00 11.72	A A
ATOM	145	N	THR A	21	25.596	34.455	14.540	1.00 14.05	A
ATOM ATOM	146 147	CA CB	THR A	21 21	25.268 24.006	34.511 33.653	13.114 12.865	1.00 12.27	A
ATOM	148	OG1	THR A	21	22.966	34.044	12.865	1.00 16.46 1.00 13.53	A A
ATOM	149	CG2	THR A	21	24.326	32.173	13.121	1.00 17.80	A
ATOM ATOM	150 151	C O	THR A	21 21	25.121 25.452	35.937 36.928	12.509 13.148	1.00 14.67 1.00 12.04	A A
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MOTA	152	N	ALA A	22	24.663	36.037	11.265	1.00 12.98	A
MOTA	153	CA	ALA A	22	24.523	37.335	10.594		
ATOM	154	CB	ALA A	22	23.913	37.146	9.208	1.00 12.25 1.00 15.06	A A
ATOM	155	С	ALA A	22	23.749	38.418	11.337	1.00 10.99	
ATOM	156	0	ALA A	22	22.688	38.174	11.916	1.00 15.12	A A
ATOM	157	N	GLY A	23	24.285	39.636	11.292	1.00 13.12	À
MOTA	158	CA	GLY A	23	23.631	40.753	11.951	1.00 14.86	A
MOTA	159	С	GLY A	23	24.068	41.057	13.371	1.00 14.00	Â
ATOM	160	0	GLY A	23	23.775	42.138	13.894	1.00 15.41	Â
ATOM	161	N	PHE A	24	24.760	40.116	14.001	1.00 12.44	A
ATOM	162	CA	PHE A	24	25.238	40.283	15.363	1.00 14.48	A
ATOM	163	CB	PHE A	24	25.424	38.899	16.020	1.00 9.89	Α
ATOM	164	CG	PHE A	24	24.156	38.276	16.527	1.00 12.35	· A
ATOM	165	CD1	PHE A	24	23.225	37.734	15.644	1.00 6.46	A
ATOM	166	CD2	PHE A	24	23.888	38.237	17.898	1.00 12.73	A
ATOM ATOM	167 168	CE1 CE2	PHE A	24	22.035	37.153	16.125	1.00 11.12	A
ATOM	169	CZ	PHE A	24 24	22.695 21.772	37.662	18.397	1.00 7.42	Ā
ATOM	170	Č	PHE A	24	26.584	37.118 41.030	17.502 15.444	1.00 11.79	A
ATOM	171	ŏ	PHE A	24	27.569	40.592	14.850	1.00 14.36 1.00 12.41	A A
ATOM	172	N	ALA A	25	26.630	42.141	16.183	1.00 14.60	A
ATOM	173	CA	ALA A	25	27.881	42.875	16.378	1.00 13.54	Ä
MOTA	174	CB	ALA A	25	27.606	44.233	17.024	1.00 15.19	A
ATOM	175	С	ALA A	25	28.752	42.031	17.315	1.00 12.48	A
ATOM	176	0	ALA A	25	28.240	41.155	18.023	1.00 12.61	A
ATOM	177	Ŋ	PRO A	26	30.067	42.289	17.348	1.00 11.27	A
MOTA	178	CD	PRO A	26	30.837	43.202	16.476	1.00 13.96	A
ATOM ATOM	179	CA	PRO A	26	30.952	41.507	18.231	1.00 12.70	A
ATOM	180 181	CB CG	PRO A	26 26	32.334	42.117	17.989	1.00 14.99	Ą
ATOM	182	c	PRO A	26	32.241	42.582 41.602	16.519	1.00 19.22	A
ATOM	183	ŏ	PRO A	26	30.222	42.681	19.699 20.192	1.00 10.57 1.00 10.54	A
ATOM	184	Ň	TYR A	27	30.529	40.456	20.367	1.00 10.54	A A
MOTA	185	CA	TYR A	27	30.161	40.345	21.793	1.00 9.13	Ä
ATOM	186	CB	TYR A	27	30.294	38.886	22.231	1.00 8.74	A
MOTA	187	CG	TYR A	27	29.824	38.612	23.648	1.00 5.12	A
MOTA	188	CD1	TYR A	27	28.469	38.512	23.938	1.00 6.81	A
ATOM	189	CE1	TYR A	27	28.024	38.224	25.247	1.00 9.00	A
ATOM	190	CD2	TYR A	27	30.741	38.423	24.682	1.00 5.70	A
ATOM	191	CE2	TYR A	27	30.310	38.131	25.992	1.00 7.78	A
ATOM ATOM	192 193	CZ OH	TYR A	27 27	28.948	38.032	26.259	1.00 9.36	Ā
ATOM	194	C	TYR A	27	28.502 31.081	37.709 41.207	27.532 22.675	1.00 8.37 1.00 10.49	A
ATOM	195	ŏ	TYR A	27	32.297	41.207	22.494	1.00 10.49	A A
ATOM	196	N	ILE A	28	30.510	41.931	23.635	1.00 8.97	Ä
ATOM	197	CA	ILE A	28	31.324	42.765	24.517	1.00 12.31	A
ATOM	198	CB	ILE A	28	30.801	44.225	24.521	1.00 13.61	A
ATOM	199	CG2	ILE A	28	31.657	45.098	25.459	1.00 13.95	A
ATOM	200	CG1	ILE A	28	30.871	44.793	23.095	1.00 11.91	A
ATOM	201	CD1	ILE A	28	30.192	46.146	22.915	1.00 12.92	A
ATOM ATOM	202 203	C O	ILE A	28	31.333	42.191	25.942	1.00 13.14	A
ATOM	203	N	ILE A GLY A	28 29	30.315 32.499	42.189 41.706	26.622 26.373	1.00 8.79 1.00 13.23	A A
ATOM	205	CA	GLY A	29	32.630	41.105	27.695	1.00 15.23	A
ATOM	206	č	GLY A	29	32.868	42.127	28.791	1.00 16.10	Ä
ATOM	207	Ō	GLY A	29	33.915	42.794	28.826	1.00 12.27	A
ATOM	208	N	THR A	30	31.900	42.234	29.697	1.00 8.70	A
ATOM	209	CA	THR A	30	31.966	43.200	30.783	1.00 10.71	A
ATOM	210	CB	THR A	30	31.061	44.442	30.473	1.00 11.83	A
ATOM	211	OG1	THR A	30	29.703	44.014	30.222	1.00 16.91	A
ATOM	212	CG2	THR A	30	31.607	45.235	29.249	1.00 8.83	A
ATOM	213 214	Č	THR A	30	31.538	42.640	32.147	1.00 11.78	A
ATOM ATOM	215	O N	THR A GLY A	30 31	31.532 31.187	43.378	33.135	1.00 11.34	A
ATOM	216	CA	GLY A	31	30.729	41.352 40.789	32.210 33.473	1.00 10.41 1.00 8.40	A A
ATOM	217	C	GLY A	31	29.208	40.604	33.467	1.00 9.64	A
ATOM	218	ŏ	GLY A	31	28.478	41.396	32.862	1.00 8.01	Â
ATOM	219	Ň	SER A	32	28.718	39.566	34.138	1.00 7.93	Ä
ATOM	220	CA	SER A	32	27.274	39.297	34.143	1.00 4.39	Ā
ATOM	221	CB	SER A	32	26.961	37.954	34.832	1.00 2.86	A
ATOM	222	OG	SER A	32	27.538	36.876	34.125	1.00 6.73	A
ATOM	223	Ç	SER A	32	26.440	40.386	34.793	1.00 7.61	A
ATOM	224	0	SER A	32	25.321	40.626	34.354	1.00 9.70	A
ATOM	225	N	GLY A	33	26.984	41.052	35.811	1.00 8.20	A
ATOM	226	CA	GLY A	33	26.256	42.121	36.506	1.00 6.91	A

MOTA	227	C	GLY	Α	33	25.942	43.235	35.524	1.00 9.1	.6 A
ATOM	228	0	GLY	Α	33	24.799	43.708	35.429	1.00 9.9	5 A
ATOM	229	N	LYS		34	26.943	43.633	34.749	1.00 10.6	
ATOM	230	CA	LYS		34	26.710	44.681	33.758	1.00 8.5	
ATOM ATOM	231 232	CB CG	LYS LYS		34	28.040	45.240	33.250	1.00 7.0	_
ATOM	233	CD	LYS	Α	34 34	28.667 29.957	46.220 46.854	34.250	1.00 12.8	
ATOM	234	CE	LYS		34	30.597	47.768	33.703 34.748	1.00 10.6 1.00 10.9	
ATOM	235	NZ	_	A	34	29.700	48.890	35.066	1.00 23.4	
MOTA	236	C	LYS		34	25.848	44.201	32.601	1.00 12.9	
ATOM	237	0	LYS		34	25.070	44.977	32.043	1.00 9.5	
ATOM ATOM	238 239	N CA	GLY GLY		35 35	25.983	42.928	32.236	1.00 9.6	
ATOM	240	C	GLY		35	25.158 23.677	42.386 42.414	31.162 31.542	1.00 7.5 1.00 9.6	
MOTA	241	ō	GLY		35	22.831	42.767	30.717	1.00 9.6 1.00 9.0	
ATOM	242	N	LYS		36	23.340	42.077	32.787	1.00 8.5	
ATOM	243	CA	LYS		36	21.929	42.089	33.173	1.00 7.2	6 A
ATOM ATOM	244 245	CB CG		A	36	21.709	41.393	34.533	1.00 9.1	_
ATOM	245	CD	LYS	A A	36 36	21.954 21.394	39.861 39.069	34.445 35.662	1.00 5.2	
ATOM	247	ČE		A	36	21.990	39.576	36.986	1.00 6.8 1.00 11.5	
ATOM	248	NZ	LYS	Α	36	21.397	38.945	38.221	1.00 11.9	
ATOM	249	Č	LYS		36	21.409	43.527	33.204	1.00 11.1	
ATOM ATOM	250	O		A	36	20.311	43.787	32.724	1.00 14.0	
ATOM	251 252	N CA	ILE		37 37	22.190 21.752	44.459 45.854	33.749	1.00 9.1	_
ATOM	253	CB		A	37	22.778	46.779	33.766 34.462	1.00 11.1	
ATOM	254	CG2		A	37	22.424	48.252	34.197	1.00 11.3	
MOTA	255	CG1		A	37	22.774	46.522	35.972	1.00 9.5	
ATOM ATOM	256	CD1		À	37	24.024	47.029	36.669	1.00 15.6	
ATOM	257 258	C	ILE	A N	37 37	21.563 20.570	46.368 47.017	32.325	1.00 11.7	
ATOM	259	Ŋ	ALA		38	22.518	46.071	32.018 31.452	1.00 11.3 1.00 9.3	
ATOM	260	CA	ALA		38	22.438	46.539	30.063	1.00 10.1	
ATOM	261	CB	ALA		38	23.650	46.016	29.269	1.00 10.9	
ATOM ATOM	262	C	ALA		38	21.129	46.102	29.375	1.00 9.6	
ATOM	263 264	O N	ALA PHE	A	38 39	20.447 20.771	46.899 44.831	28.712 29.541	1.00 8.4	
ATOM	265	CA		À	39	19.566	44.327	28.914	1.00 8.7 1.00 9.4	
ATOM	266	CB		Α	39	19.549	42.787	28.888	1.00 9.0	
MOTA	267	CG		A	39	18.287	42.214	28.270	1.00 7.1	6 A
ATOM ATOM	268 269	CD1 CD2		A A	39	18.223	41.953	26.896	1.00 8.5	
ATOM	270	CE1	PHE		39 39	17.146 17.035	42.000 41.481	29.051 26.306	1.00 8.1 1.00 9.1	
ATOM	271	CE2		A	39	15.947	41.530	28.479	1.00 9.0	
ATOM	272	CZ		A	39	15.888	41.269	27.101	1.00 8.2	
ATOM ATOM	273	C	PHE.		39	18.304	44.790	29.608	1.00 12.1	
ATOM	274 275	N O	PHE .	Α	39 40	17.398 18.246	45.313 44.602	28.972 30.920	1.00 10.7	
ATOM	276	CA	LEU		40	17.034	44.938	31.678	1.00 8.7 1.00 8.9	
MOTA	277	CB	LEU .		40	17.204	44.513	33.144	1.00 7.8	
ATOM	278	CG.		A	40	17.342	43.005	33.400	1.00 10.0	
ATOM ATOM	279 280		LEU .	A A	40 40	17.809	42.781	34.887	1.00 6.4	
ATOM	281	CDZ	LEU .		40	16.006 16.626	42.296 46.403	33.132	1.00 12.5	
ATOM	282	ŏ	LEU		40	15.430	46.730	31.632	1.00 10.6	
MOTA	283	N	GLU .		41	17.604	47.291	31.586	1.00 10.8	
MOTA	284	CA	GLU .		41	17.294	48.717	31.551	1.00 9.1	
ATOM ATOM	285 286	CB CG	GLU .		41 41	18.053 17.802	49.436	32.669	1.00 13.2	
ATOM	287	CD	GLU :		41	18.671	48.829 49.429	34.036 35.131	1.00 11.0 1.00 22.5	
ATOM	288		GLU .		41	18.975	48.713	36.103	1.00 27.3	
ATOM	289	OE2	GLU 3	A	41	19.037	50.616	35.043	1.00 22.4	
ATOM	290	C	GLU A		41	17.633	49.361	30.218	1.00 12.7	2 A
ATOM ATOM	291 292	O N	GLU A		41 42	17.505 18.010	50.576	30.066	1.00 13.6	
ATOM	293	CA	ASN A		42	18.463	48.537 49.008	29.238 27.923	1.00 11.7	
ATOM	294	CB	ASN A		42	17.322	49.494	27.022	1.00 11.7	
MOTA	295	CG	ASN A	A	42	17.824	49.897	25.642	1.00 16.5	
ATOM	296		ASN A		42	18.885	49.428	25.189	1.00 15.6	7 A
ATOM ATOM	297 298	ND2 C	ASN A		42 42	17.076	50.763	24.960	1.00 14.2	
ATOM	299	ŏ	ASN A		42	19.486 19.300	50.126 51.260	28.091 27.631	1.00 16.60	
ATOM	300	Ň	SER A		43	20.578	49.789	28.767	1.00 14.5	

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21.665 50.740 29.001 1.00 14.54 MOTA 301 CA SER A 43 1.00 19.90 MOTA 302 CB SER A 21.920 50.874 30.520 43 MOTA 31.162 1.00 26.26 303 SER A 20.922 51.662 13.78 28.302 1.00 MOTA 304 SER A 43 22.965 50.327 MOTA 305 SER A 49.633 28.891 1.00 10.60 43 27.056 1.00 MOTA 306 TYR A 23.168 50.755 44 1.00 26.361 10.86 MOTA 307 CA TYR A 44 24.396 50.401 CB MOTA 308 TYR A 44 24.330 50.880 24.904 1.00 10.54 309 CG TYR 44 25.414 50.311 24.034 1.00 MOTA 26.631 27.625 310 CD1 TYR A 50.983 23.857 1.00 ATOM 44 CE1 TYR A 23.011 311 50.469 1.00 10.91 MOTA 44 CD2 CE2 25.217 26.201 49.106 23.357 1.00 10.34 TYR A 44 MOTA 312 22.517 313 TYR A 48.587 1.00 11.21 ATOM 44 27.394 28.357 22.347 21.524 27.026 TYR A CZ OH 49.267 48.725 1.00 MOTA 314 44 14.12 1.00 11.54 44 MOTA 315 44 25.650 26.775 50.971 1.00 8.02 Α **ATOM** 316 c TYR A 26.756 27.917 50.515 1.00 10.36 TYR A MOTA 317 44 25.484 26.657 1.00 8.55 A MOTA 318 И ASN A 45 51.941 28.535 29.337 30.708 1.00 14.36 CA 52.547 MOTA 319 ASN Α 45 26.271 25.707 A CB 1.00 45 53.811 8.69 MOTA 320 ASN A ASN A 53.503 11.69 A MOTA 321 CG 45 1.00 25.048 MOTA 322 OD1 ASN A 45 52.488 30.910 1.00 13.56 Α MOTA 323 ND2 ASN Α 45 25.934 54.411 31.655 1.00 14.48 29.388 29.755 27.423 A MOTA 324 ASN A 45 51.535 1.00 13.91 51.781 325 0 ASN A 45 28.573 1.00 11.13 A MOTA 26.788 27.462 29.681 MOTA 326 N GLN A 46 50.393 1.00 8.83 327 CA GLN A 46 49.337 30.435 1.00 11.62 MOTA 26.421 25.487 328 CB GLN A 46 48.390 31.080 1.00 10.13 ATOM MOTA CG GLN Α 46 49.076 32.083 1.00 14.66 ATOM 330 CD GLN A 46 26.259 49.792 33.170 1.00 18.72 OE1 GLN Α٠ 46 26.983 49.165 33.937 1.00 18.65 MOTA 331 NE2 GLN A 46 26.133 51.116 33.228 1.00 16.99 MOTA 332 333 GLN A 46 28.408 48.543 29.491 1.00 10.06 MOTA 29.275 28.232 GLN A 46 47.818 29.956 1.00 10.43 **ATOM** 334 N PHE Α 47 48.691 28.174 1.00 8.72 MOTA 335 CA PHE A 47 29.055 48.025 27.148 1.00 7.46 ATOM 336 CB PHE A 47 28.191 47.487 25.992 1.00 7.56 MOTA 337 26.366 27.559 1.00 MOTA 338 CG PHE A 47 27.271 46.349 12.11 45.651 45.945 **ATOM** 339 CD1 PHE A 47 27.433 1.00 11.35 CD2 47 26.268 25.474 1.00 14.21 MOTA 340 PHE A 44.567 27.861 1.00 ATOM 341 CE1 PHE A 47 26.616 1.00 PHE A 47 25.442 44.859 25.761 9.84 MOTA 342 CE2 25.617 44.167 26.959 1.00 10.19 MOTA 343 CZPHE A 47 1.00 Ĉ 47 30.053 48.988 26.484 12.94 ATOM 344 PHE A 26.022 ATOM 345 0 PHE A 47 31.109 48.580 1.00 14.11 29.677 50.257 26.378 1.00 11.49 MOTA 346 . N GLY A 48 30.551 ATOM 347 CA GLY A 48 51.222 25.731 1.00 13.51 15.44 348 č GLY A 48 52.642 25.833 1.00 ATOM 52.908 0 GLY A 48 28.999 26.459 1.00 16.60 ATOM 349 30.722 53.566 25.187 1.00 350 N THR A 49 14.37 ATOM 30.333 25.256 1.00 13.58 CA CB THR A 49 54.967 ATOM 351 31.576 55.843 25.161 THR A 49 1.00 14.46 MOTA 352 55.567 55.524 49 23.924 1.00 15.00 ATOM 353 OG1 THR A 32.558 THR A 26.322 1.00 13.17 354 CG2 49 ATOM 29.301 28.716 1.00 55.436 24.216 14.30 A THR A 49 MOTA 355 С 24.370 1.00 12.47 56.511 MOTA 356 0 THR A 49 1.00 13.09 29.062 54.659 23.162 MOTA 357 N ASN A 50 22.173 20.785 19.739 28.076 55.116 1.00 14.85 MOTA 358 CA ASN A 50 1.00 15.63 28.324 27.379 54.519 **ATOM** 359 CB ASN A 50 55.096 55.883 18.88 MOTA 360 CG ASN A 50 1.00 26.472 27.574 20.059 1.00 ATOM 361 OD1 ASN A 50 19.28 18.489 19.28 MOTA 362 ND2 ASN A 50 54.707 1.00 22.615 22.187 1.00 14.82 MOTA 363 ASN A 50 26.669 54.751 53.739 14.58 364 0 ASN A 50 26.099 1.00 ATOM 365 THR A 51 26.097 55.608 23.443 1.00 13.25 ATOM 15.77 THR A 51 24.782 55.377 23.988 1.00 MOTA 366 25.242 24.973 CB THR A 24.595 56.210 1.00 17.96 MOTA 367 **ATOM** 368 OG1 THR A 51 24.937 57.574 1.00 16.18 369 CG2 THR A 25.506 55.684 26.332 1.00 18.64 MOTA 23.581 55.539 23.053 1.00 18.71 370 C THR A 51 ATOM 23.512 371 ō THR A 51 22.440 55.436 1.00 19.68 ATOM 55.795 21.761 1.00 372 52 23.820 16.82 ATOM N THR A 55.865 20.827 19.67 373 CA THR A 52 22.702 1.00 MOTA 52 23.017 56.666 19.524 1.00 22.55 CB THR A ATOM 374 18.744 THR 52 24.028 56.006 1.00 ATOM 375 OG1

ATOM	376	CG2	THR A	52	23.460	58.081	19.875	1.00 21.07	Α
ATOM	377	C	THR A	52	22.342	54.428	20.446	1.00 17.92	A
ATOM	378	0	THR A	52	21.270	54.175	19.905	1.00 17.96	A
ATOM ATOM	379 380	N CA	LYS A LYS A	53 53	23.238	53.488	20.740	1.00 14.41	A
ATOM	381	CB	LYS A	53 53	22.978 24.292	52.080 51.292	20.427 20.406	1.00 12.53	A
ATOM	382	CG	LYS A	53	25.207	51.573	19.213	1.00 14.33 · 1.00 17.93	A A
ATOM	383	CD	LYS A	53	26.478	50.731	19.324	1.00 18.20	Ä
ATOM	384	CE	LYS A	53	27.477	51.052	18.214	1.00 21.01	A
ATOM ATOM	385 386	NZ C	LYS A LYS A	53 53	26.908	50.784	16.865	1.00 22.67	A
ATOM	387	ŏ	LYS A	53 53	22.045 22.075	51.470 51.869	21.474 22.635	1.00 12.72 1.00 11.93	A A
ATOM	388	N	ASP A	54	21.223	50.499	21.064	1.00 13.58	A
ATOM	389	CA	ASP A	54	20.298	49.826	21.982	1.00 10.96	A
ATOM ATOM	390 391	CB	ASP A	54 .	18.887	49.745	21.380	1.00 12.81	A
ATOM	392	CG OD1	ASP A ASP A	54 54	18.249 18.010	51.107 51.529	21.218 20.059	1.00 19.07 1.00 17.31	A
ATOM	393	OD2		54	17.997	51.759	22.260	1.00 17.31	A A
ATOM	394	Ç	ASP A	54	20.819	48.416	22.246	1.00 8.44	A
ATOM	395	O.	ASP A	54	21.505	47.837	21.407	1.00 14.56	A
ATOM ATOM	396 397	N CA	VAL A VAL A	55 55	20.485 20.919	47.875 46.541	23.411 23.799	1.00 12.75 1.00 12.22	A
ATOM	398	CB	VAL A	55	21.150	46.486	25.328	1.00 12.22 1.00 7.89	A A
MOTA	399	CG1	VAL A	55	21.596	45.057	25.775	1.00 7.35	A
ATOM	400	CG2	VAL A	55	22.229	47.518	25.707	1.00 6.23	A
ATOM ATOM	401 402	C O	VAL A VAL A	55 55	19.840 18.659	45.540 45.768	23.386	1.00 9.36	A
ATOM	403	Ŋ	HIS A	56	20.258	44.441	23.630 22.755	1.00 11.95 1.00 9.82	A A
ATOM	404	CA	HIS A	56	19.323	43.432	22.285	1.00 8.89	Ä
ATOM	405	CB	HIS A	56	19.552	43.218	20.782	1.00 8.33	A
ATOM ATOM	406 407	CC	HIS A HIS A	56 56	19.455° 20.414	44.485 45.264	19.985 19.430	1.00 9.48	A
ATOM	408	ND1	HIS A	56	18.255	45.121	19.738	1.00 11.14 1.00 13.82	A A
ATOM	409		HIS A	56	18.483	46.236	19.064	1.00 12.14	A
ATOM	410	NE2		56	19.783	46.345	18.866	1.00 12.83	A
ATOM ATOM	411 412	С 0	HIS A	56 56	19.389 18.419	42.097 41.331	23.033 23.039	1.00 9.87 1.00 8.84	A A
ATOM	413	Ň	TRP A	57	20.531	41.797	23.649	1.00 10.03	A
MOTA	414	CA	TRP A	57	20.618	40.535	24.385	1.00 12.07	A
ATOM	415	CB	TRP A	57	20.753	39.340	23.430	1.00 7.72	A
ATOM ATOM	416 417	CG CD2	TRP A	57 57 .	22.078 23.188	39.288 38.398	22.673 22.935	1.00 9.96 1.00 8.55	A A
ATOM	418	CE2	TRP A	57	24.161	38.642	21.945	1.00 7.37	Â
MOTA	419	CE3	TRP A	57	23.442	37.413	23.914	1.00 9.79	A
ATOM	420	CD1	TRP A	57	22.430	40.021	21.570	1.00 9.43	A
ATOM ATOM	421 422	NE1 CZ2	TRP A	57 57	23.685 25.381	39.637 37.936	21.124 21.895	1.00 7.89 1.00 8.66	A A
ATOM	423	CZ3	TRP A	57	24.647	36.713	23.862	1.00 7.59	Ä
ATOM	424	CH2	TRP A	57	25.605	36.982	22.852	1.00 13.66	A
ATOM ATOM	425 426	C	TRP A	57 57	21.830 22.648	40.575 41.481	25.286 25.179	1.00 9.35	A
ATOM	427	Ŋ	ALA A	58	21.945	39.579	26.159	1.00 9.06 1.00 6.35	A A
ATOM	428	CA	ALA A	58	23.081	39.523	27.061	1.00 8.26	Ä
ATOM	429	CB	ALA A	58	22.755	40.280	28.362	1.00 10.03	Ā
ATOM ATOM	430 431	C O	ALA A ALA A	58 58	23.471 22.638	38.101 37.207	27.407 27.401	1.00 7.97 1.00 9.27	A A
ATOM	432	Ň	GLY A	59	24.749	37.908	27.702	1.00 9.58	Â
ATOM	433	CA	GLY A	59	25.213	36.608	28.184	1.00 7.09	A
MOTA	434	Č	GLY A	59 50	25.342	36.791	29.695	1.00 9.23	A
ATOM ATOM	435 436	O N	GLY A SER A	59 60	25.779 24.938	37.846 35.801	30.159 30.484	1.00 10.14 1.00 5.73	A A
ATOM	437	CA	SER A	60	25.058	35.917	31.938	1.00 5.95	A
MOTA	438	CB	SER A	60	23.815	36.613	32.535	1.00 10.17	A
ATOM	439	og	SER A	60	23.896	36.707	33.966	1.00 9.12	A
ATOM ATOM	440 441	C	SER A SER A	60 60	25.161 24.437	34.540 33.632	32.566 32.146	1.00 8.54 1.00 9.12	A A
MOTA	442	Ň	ASP A	61	26.067	34.376	33.536	1.00 9.30	Â
ATOM	443	CA	ASP A	61	26.132	33.124	34.292	1.00 8.23	A
ATOM	444	CB	ASP A	61	27.543	32.485	34.381	1.00 6.13	A
ATOM ATOM	445 446	CG OD1	ASP A ASP A	61 61	28.600 28.869	33.266 32.961	33.649 32.449	1.00 13.41 1.00 10.15	A A
ATOM	447	OD2	ASP A	61	29.150	34.191	34.281	1.00 13.11	Ä
MOTA	448	С	ASP A	61	25.597	33.456	35.710	1.00 10.77	A
MOTA	449	0	ASP A	61	25.818	32.716	36.658	1.00 11.14	A
MOTA MOTA	450 451	N CA	SER A SER A	62 62	24.914 24.213	34.595 34.995	35.833 37.067	1.00 7.59 1.00 10.29	A A
.11011	- J -	CA	J 11				2	2.00 10.27	

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ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	23345678901234567890012345678900123456789001234567890012345678900123456789001234567890012345678900123456789001234567890012345678900123456789001234567890012345678900123456789000000000000000000000000000000000000	CD2 C O N CA CB C O N CA CB OG1 CG2 C	A A A A A A A A A A A A A A A A A A A	66666666666666666666666666666666666666	24.521 22.2744 22.2744 22.2744 21.944 20.519 19.148 17.7986 19.149 19.149 19.149 19.149 11.589 11.686 17.150 11.7.150 11.7.150 11.7.150 11.7.150 11.7.150 11.8.649 11.8.23 11.8.33 11.8.33 11.8.40 11.8.40 11.8.659 11.8.65	72445896591782346896541221111188458333333333333333333333333333333	79965979118997992465000788241255931171594667842245503569711844849772277996597997992465000078241255933133333333333333333333333333333333	1.00 11.42 1.00 11.94 1.00 10.70 1.00 9.88 1.00 10.63 1.00 16.43 1.00 15.34 1.00 16.96 1.00 14.00 1.00 17.10 1.00 7.71 1.00 9.01 1.00 9.01 1.00 10.37 1.00 9.71 1.00 10.37 1.00 10.36 1.00 10.36 1.00 11.54 1.00 13.32 1.00 12.42 1.00 12.43 1.00 12.43 1.00 12.31 1.00 12.31 1.00 12.31 1.00 13.43 1.00 13.43 1.00 13.43 1.00 12.44 1.00 13.43 1.00 13.43	AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	517 518 519 520 521 522 523 524 525 526	CG2 C O N CA CB CG CD1 CE1 CD2	THR A THR A THR A TYR A	71 71 72 72 72 72 72 72 72 72	12.225 10.501 9.881 11.116 11.049 11.927 12.194 13.122 13.376 11.515	46.811 44.905 45.800 43.941 43.941 42.839 43.011 43.936 44.101 42.239	37.267 35.902 35.337 35.223 33.760 33.174 31.682 31.224 29.841 30.736	1.00 13.43 1.00 11.57 1.00 15.24 1.00 13.13 1.00 12.95 1.00 11.21 1.00 12.14 1.00 11.17 1.00 11.35 1.00 14.03	A A A A A A A
MOTA	527	CE2	TYR A	72	11.765	42.378	29.372	1.00 8.40	A

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ATOM	528	CZ	TYR	λ	72	12 600	42 202	20 020	1 00 10 10	
		_				12.689	43.303	28.928	1.00 10.19	A
ATOM	529	ОН	TYR		72	12.949	43.425	27.585	1.00 10.75	A
ATOM	530	C	TYR	A	72	9.604	43.705	33.313	1.00 13.42	A
ATOM	531	0	TYR	A	72	9.111	44.346	32.394	1.00 14.74	A
MOTA	532	N	ALA		73	8.943	42.763	33.970		
ATOM	533	CA							1.00 14.68	A
			ALA		73	7.563	42.423	33.650	1.00 15.37	A
ATOM	534	CB	ALA	Α	73	7.090	41.293	34.556	1.00 10.74	A
ATOM	535	С	ALA	A	73	6.631	43.626	33.791	1.00 14.04	. A
ATOM	536	0	ALA	Δ	73	5.711	43.811	32.992	1.00 13.32	A
ATOM	537	Ň	ALA		74					
						6.856	44.436	34.815	1.00 16.88	A
ATOM	538	CA	ALA		74	6.006	45.602	35.032	1.00 17.08	A
ATOM	539	CB	ALA	Α	74	6.082	46.052	36.505	1.00 13.94	A
MOTA	540	С	ALA	Α	74	6.354	46.768	34.118	1.00 20.94	A
ATOM	541	0	ALA		74	5.475	47.357	33.476	1.00 17.04	A
ATOM	542	Ň	ASN							
					75	7.645	47.061	34.014	1.00 15.74	A
ATOM	543	CA	ASN		75	8.125	48.203	33.241	1.00 17.76	A
ATOM	544	CB	ASN	Α	75	9.439	48.712	33.839	1.00 19.52	A
ATOM	545	CG	asn	Α	75	9.308	49.152	35.289	1.00 24.86	A
ATOM	546	OD1	ASN	Α	75	10.308	49.485	35.929	1.00 26.13	A
ATOM	547	ND2	ASN		75	8.084	49.150	35.816		
									1.00 27.41	A
ATOM	548	C	ASN		75	8.356	48.070	31.741	1.00 18.90	A
ATOM	549	0	ASN		75	8.049	48.996	30.986	1.00 16.37	A
MOTA	550	N	LYS	Α	76	8.910	46.944	31.304	1.00 13.20	Α
ATOM	551	CA	LYS	A	76	9.235	46.810	29.888	1.00 14.05	Α
ATOM	552	CB	LYS	Α	76	10.709	46.412	29.730	1.00 11.81	A
ATOM	553	ĊĠ			76	11.706	47.189	30.561	1.00 15.12	Ä
ATOM	554	CD			76					
						11.710	48.673	30.208	1.00 18.17	A
ATOM	555	CE			76	12.942	49.342	30.783	1.00 21.75	A
ATOM	556	NZ			76	12.858	50.832	30.665	1.00 23.76	A
ATOM	557	С	LYS	Α	76	8.414	45.835	29.064	1.00 14.89	A
ATOM	558	0	LYS	A	76	8.184	46.053	27.874	1.00 15.18	A
ATOM	559	N	GLN		77	7.996	44.746	29.686	1.00 13.65	A
ATOM	560	ĊA	GLN		77	7.240	43.718			
ATOM								28.978		A
	561	CB	GLN		77	6.865	42.625	29.964	1.00 14.98	A
ATOM	562	CG	GLN		77	6.139	41.438	29.381	1.00 18.91	Α
ATOM	563	CD	GLN	A	77	5.848	40.392	30.441	1.00 26.71	Α
ATOM	564	OE1	GLN	A	77	6.747	39.965	31.167	1.00 25.14	A
ATOM	565	NE2	GLN .	Α	77	4.593	39.968	30.534	1.00 21.79	A
ATOM	566	C	GLN		77	5.989	44.205	28.222	1.00 16.81	
ATOM	567		GLN		ήή					A
		Ö.				5.718	43.746	27.114	1.00 17.54	Α
ATOM	568	N	PRO .		78	5.216	45.142	28.800	1.00 19.48	A
ATOM	569	CD	PRO	A	78	5.255	45.765	30.134	1.00 12.68	A
ATOM	570	CA	PRO .	A	78	4.023	45.575	28.056	1.00 15.54	A
ATOM	571	CB	PRO .	A '	78	3.428	46.654	28.958	1.00 19.25	Ä
ATOM	572	CG	PRO .		78	3.787	46.150	30.342	1.00 17.82	Ä
ATOM	573	Č	PRO .		78	4.325	46.080			
ATOM	574							26.646	1.00 20.10	A
		Ö.	PRO .		78	3.614	45.748	25.692	1.00 18.30	Α
MOTA	575	N	GLY .		79	5.393	46.860	26.512	1.00 15.27	A
ATOM	576	CA	GLY .	A '	79	5.745	47.379	25.210	1.00 17.02	A
ATOM	577	С	GLY .	A '	79	6.802	46.616	24.427	1.00 20.02	A
ATOM	578	0	GLY .	A '	79	6.839	46.731	23.199	1.00 15.38	A
ATOM	579	N	TRP .	A :	80	7.639	45.830	25.111	1.00 13.75	Ä
ATOM	580	CA			80	8.723	45.092	24.440	1.00 14.43	Ä
ATOM	581	CB			80			25.136		
						10.062	45.359		1.00 11.39	A
ATOM	582	CG			80	10.549	46.780	25.071	1.00 15.13	A
ATOM	583		TRP .		80	11.672	47.329	25.767	1.00 13.37	Α
ATOM	584		TRP .		80	11.823	48.666	25.332	1.00 13.52	A
ATOM	585	CE3	TRP 2	A I	80	12.573	46.817	26.716	1.00 12.51	. А
ATOM	586	CD1	TRP .	A i	80	10.068	47.779	24.271	1.00 19.04	A
ATOM	587		TRP I		80	10.831	48.919	24.418	1.00 16.58	Ä
ATOM	588	CZ2	TRP		80	12.840	49.502	25.812	1.00 15.28	
ATOM	589	CZ3	TRP			13.586				A
					80		47.645	27.197	1.00 13.05	A
ATOM	590	CH2	TRP		80	13.710	48.979	26.739	1.00 16.82	A
ATOM	591	C	TRP /	A I	80	8.560	43.580	24.349	1.00 16.83	A
ATOM	592	0	TRP A	A 8	80	9.361	42.909	23.685	1.00 16.92	A
ATOM	593	N	GLY A	A (81	7.562	43.031	25.033	1.00 15.56	A
MOTA	594	CA	GLY Z		81	7.380	41.584	25.001	1.00 11.72	Ä
ATOM	595	C	GLY 2		81	8.071	40.921	26.186	1.00 11.72	A
ATOM	596	ŏ	GLY A			8.856				
					81 82		41.557	26.894	1.00 8.85	Ā
ATOM	597	N	LYS A		82	7.784	39.638	26.395	1.00 10.46	A
MOTA	598	CA	LYS A		B2	8.374	38.882	27.499	1.00 11.96	A
ATOM	599	CB	LYS A		82	7.702	37.506	27.608	1.00 11.82	A
ATOM	600	CG	LYS A		82	6.341	37.497	28.315	1.00 12.27	A
ATOM	601	CD	LYS A	A 6	82	5.578	36.167	28.137	1.00 15.83	A
ATOM	602	CE	LYS A		82	6.296	34.971	28.782	1.00 21.44	A
ATOM	603	NZ	LYS Z		82	6.571	35.179	30.234	1.00 18.30	Ä
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ATOM	668	Ç	THR A	91	31.116	24.140	33.686	1.00 10.91	A
ATOM	671	CA	SER A	92	32.972	23.598	35.122	1.00 11.52	· A
ATOM	672 673	CB	SER A		34.167	22.642	35.011	1.00 12.03	A
ATOM ATOM	673 674	OG C	SER A		35.213 33.490	23.181 24.962	34.186 35.601	1.00 10.62 1.00 10.73	A A
ATOM	675	0	SER A	92	33.397	25.974	34.883	1.00 8.53	Α
ATOM ATOM	676 677	N CA	VAL A		33.980 34.640	25.003 26.197	36.837 37.369	1.00 8.68 1.00 7.08	A A
MOTA	678	CB	VAL A	93	34.010	26.736	38.667	1.00 7.09	A
MOTA	679	CG1	VAL A	93	34.896	27.906	39.215	1.00 10.40	A

ATOM 680 CG2 VAL A 93 32.592 27.269 38.376 1.00 10.45 ATOM 681 C VAL A 93 36.013 25.643 37.694 1.00 10.45 ATOM 682 O VAL A 93 36.162 24.745 38.527 1.00 12.26 ATOM 682 N ALIA A 94 37.064 26.148 37.025 1.00 8.00 ATOM 683 N ALIA A 94 37.064 26.148 37.025 1.00 8.00 ATOM 685 CB ALIA A 94 38.425 25.645 37.236 1.00 8.64 ATOM 686 CB ALIA A 94 38.425 25.645 37.236 1.00 7.787 ATOM 687 O ALIA A 94 38.306 27.331 38.251 1.00 7.787 ATOM 688 N LLE A 95 40.210 25.709 38.894 1.00 5.77 ATOM 689 CA ILE A 95 40.210 25.709 38.894 1.00 5.77 ATOM 689 CB ILE A 95 40.210 25.709 38.894 1.00 5.77 ATOM 699 CC ILE A 95 40.200 25.466 11.307 1.00 9.66 ATOM 691 CC ILE A 95 40.200 25.466 11.307 1.00 9.66 ATOM 692 CC ILE A 95 40.200 25.466 14.307 1.00 9.66 ATOM 693 CD ILE A 95 40.200 25.466 14.307 1.00 9.66 ATOM 694 C ILE A 95 40.200 25.466 14.307 1.00 9.66 ATOM 695 C ILE A 95 40.200 25.466 14.307 1.00 9.66 ATOM 695 C ILE A 95 40.200 25.466 14.307 1.00 9.66 ATOM 695 C ILE A 95 40.200 25.466 14.307 1.00 9.66 ATOM 695 C ILE A 95 40.200 25.466 16.201 1.00 10.131 0.00 9.40 ATOM 695 C ILE A 95 40.200 25.466 16.201 1.00 10.131 0.00 9.40 ATOM 695 C ILE A 95 40.200 25.466 16.201 1.00 10.131 0.00 9.40 ATOM 696 N PRO A 96 42.233 27.216 38.742 1.00 6.65 ATOM 697 C D PRO A 96 42.233 27.216 38.742 1.00 6.65 ATOM 698 C B PRO A 96 42.133 22.265 38.266 1.00 7.43 ATOM 699 C B PRO A 96 42.133 22.265 38.266 1.00 7.43 ATOM 699 C B PRO A 96 42.133 22.265 38.266 1.00 7.43 ATOM 699 C B PRO A 96 42.133 27.265 38.266 1.00 9.00 ATOM 700 C B POO A 96 42.133 27.265 38.266 1.00 9.00 ATOM 700 C B POO A 96 42.133 27.265 38.266 1.00 9.00 ATOM 700 C B POO A 96 42.133 27.265 38.266 1.00 9.00 ATOM 700 C B POO A 96 44.273 27.10 9.30 9.30 9.30 9.30 9.30 9.30 9.30 9.3										
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ATOM 699 CB PRO A 96 44.275 28.107 37.054 1.00 9.06 ATOM 700 CG PRO A 96 45.133 27.938 39.414 1.00 10.94 ATOM 701 C PRO A 96 45.133 27.938 39.414 1.00 10.94 ATOM 702 O PRO A 96 45.133 27.938 39.414 1.00 10.94 ATOM 703 N PHE A 97 46.441 27.715 39.447 1.00 9.05 ATOM 704 CA PHE A 97 47.276 28.302 40.480 1.00 8.97 ATOM 705 CB PHE A 97 47.276 28.302 40.480 1.00 8.97 ATOM 706 CG PHE A 97 47.259 27.414 41.732 1.00 10.70 ATOM 707 CD1 PHE A 97 47.748 26.015 41.477 1.00 9.86 ATOM 707 CD1 PHE A 97 47.748 26.015 41.477 1.00 9.86 ATOM 708 CD2 PHE A 97 49.114 25.720 41.524 1.00 10.70 ATOM 708 CD2 PHE A 97 49.114 25.720 41.524 1.00 7.97 ATOM 708 CD2 PHE A 97 49.580 24.436 41.211 1.00 7.99 ATOM 709 CEI PHE A 97 47.326 23.704 40.802 1.00 8.94 ATOM 710 CE2 PHE A 97 47.326 23.704 40.802 1.00 8.94 ATOM 711 CZ PHE A 97 48.709 23.733 40.852 1.00 7.63 ATOM 712 C PHE A 97 48.709 23.433 40.852 1.00 7.63 ATOM 713 O PHE A 97 48.698 28.418 39.949 1.00 9.55 ATOM 714 N ARC A 98 49.498 29.260 40.597 1.00 8.26 ATOM 715 CB ARC A 98 51.149 30.927 39.808 1.00 11.26 ATOM 716 CB ARC A 98 51.149 30.927 39.808 1.00 11.26 ATOM 717 CG ARC A 98 51.149 30.927 39.808 1.00 11.26 ATOM 718 CD ARC A 98 51.149 30.927 39.808 1.00 12.41 ATOM 719 CC ARC A 98 51.149 30.927 39.808 1.00 12.41 ATOM 719 CG ARC A 98 51.149 30.927 39.808 1.00 12.41 ATOM 718 CD ARC A 98 51.149 30.927 39.808 1.00 12.41 ATOM 718 CD ARC A 98 51.195 29.881 42.327 1.00 12.72 ATOM 720 CZ ARC A 98 51.955 29.881 42.327 1.00 12.72 ATOM 720 CZ ARC A 98 51.955 29.881 42.327 1.00 12.72 ATOM 721 CC ARC A 98 51.955 29.881 42.327 1.00 12.72 ATOM 722 C LYS A 99 53.081 27.314 42.510 1.00 11.76 ATOM 723 C LYS A 99 53.081 27.314 42.510 1.00 11.72 ATOM 724 C ARC A 98 51.955 29.881 42.327 1.00 12.72 ATOM 725 C LYS A 99 53.809 26.095 41.956 1.00 11.76 ATOM 736 C B ALA A 100 55.920 23.987 43.303 1.00 16.53 ATOM 737 C C LYS A 99 53.899 26.491 44.919 1.00 13.72 ATOM 740 C C LYS A 99 53.899 26.095 41.956 1.00 11.78 ATOM 740 C C LYS A 99 53.899 26.095 41.956 1.00 11.78 ATOM 740 C C LYS A 99 53.895 20.999 44.11.19								38.063	1.00 6.16	A
ATOM 700 CG PRO A 96	MOTA		CA	PRO A	96	44.330	27.265	38.326	1.00 7.43	A
ATOM 702 C PRO A 96 45.133 27.938 39.434 1.00 10.94 ATOM 703 N PHE A 97 46.441 27.715 39.447 1.00 9.05 ATOM 704 CA PHE A 97 46.441 27.715 39.447 1.00 9.05 ATOM 705 CB PHE A 97 47.276 28.302 40.480 1.00 8.21 ATOM 706 CG PHE A 97 47.276 28.302 40.480 1.00 8.97 ATOM 706 CG PHE A 97 47.275 27.414 41.732 1.00 10.70 ATOM 707 CD1 PHE A 97 47.748 26.015 41.477 1.00 9.86 ATOM 708 CD2 PHE A 97 49.114 25.720 41.524 1.00 10.13 ATOM 708 CD2 PHE A 97 49.114 25.720 41.524 1.00 10.13 ATOM 709 CE1 PHE A 97 49.589 24.436 41.211 1.00 7.97 ATOM 709 CE2 PHE A 97 49.589 24.436 41.211 1.00 7.97 ATOM 710 CE2 PHE A 97 47.326 23.704 40.802 1.00 7.63 ATOM 711 CZ PHE A 97 48.698 24.436 41.211 1.00 7.95 ATOM 712 C PHE A 97 48.698 28.418 39.949 1.00 9.55 ATOM 713 O PHE A 97 49.589 24.436 41.211 1.00 9.55 ATOM 714 N ARCA A 98 49.498 29.260 40.597 1.00 8.26 ATOM 715 CA ARCA A 98 50.900 29.457 40.205 1.00 11.26 ATOM 716 CB ARCA A 98 50.900 29.457 40.205 1.00 11.26 ATOM 717 CG ARCA A 98 51.149 30.927 39.808 1.00 13.41 ATOM 718 CD ARCA A 98 52.902 32.648 39.002 1.00 12.41 ATOM 719 NE ARCA A 98 52.902 32.648 39.002 1.00 12.41 ATOM 720 CZ ARCA A 98 55.048 33.714 39.670 1.00 10.605 ATOM 721 NH1 ARCA A 98 55.048 33.714 39.670 1.00 10.605 ATOM 722 NH2 ARCA A 98 55.048 33.714 39.670 1.00 10.605 ATOM 722 C ARCA A 98 55.048 33.714 39.670 1.00 10.605 ATOM 722 C ARCA A 98 55.048 33.714 39.670 1.00 12.41 ATOM 722 C ARCA A 98 51.955 29.881 42.327 1.00 12.72 ATOM 724 C ARCA A 98 51.955 29.881 42.327 1.00 12.72 ATOM 725 C ARCA A 99 53.081 27.314 42.510 1.00 10.605 ATOM 726 C ARCA A 99 53.081 27.314 42.510 1.00 10.605 ATOM 727 CB LYS A 99 53.081 27.314 42.510 1.00 10.62 ATOM 727 CB LYS A 99 53.081 27.314 42.510 1.00 10.62 ATOM 726 C ARCA A 98 51.955 29.881 42.327 1.00 12.72 ATOM 727 CB LYS A 99 53.081 27.314 42.510 1.00 10.62 ATOM 727 CB LYS A 99 53.081 27.314 42.510 1.00 10.62 ATOM 730 C C LYS A 99 53.899 26.095 41.956 1.00 11.78 ATOM 740 C C ARCA A 100 55.920 23.990 44.914 1.00 10.16.53 ATOM 740 C C LYS A 99 53.809 26.095 41.956 1.00 11.78 ATOM 741 C C ARCA	MOTA	699	CB	PRO A	96	44.275	28.107	37.054	1.00 9.06	A
ATOM 703 N PHE A 97	MOTA	700	CG	PRO A	96	43.207	29.147	37.446	1.00 8.84	A
ATOM 703 N PHE A 97	MOTA	701	C	PRO A	96	45.133	27.938	39.434	1.00 10.94	A
ATOM 704 CA PHE A 97	MOTA	702	0	PRO A	96					A
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ATOM 705 CB PHE A 97 47.259 27.414 41.732 1.00 10.70 ATOM 706 CG PHE A 97 47.748 26.015 41.477 1.00 9.86 ATOM 707 CD1 PHE A 97 49.114 25.720 41.524 1.00 10.13 ATOM 708 CD2 PHE A 97 46.862 25.010 41.121 1.00 7.97 ATOM 709 CE1 PHE A 97 46.862 25.010 41.121 1.00 7.97 ATOM 710 CE2 PHE A 97 49.589 24.436 41.211 1.00 7.97 ATOM 710 CE2 PHE A 97 47.326 23.704 40.802 1.00 8.94 ATOM 711 CZ PHE A 97 48.698 23.433 40.852 1.00 7.63 ATOM 712 C PHE A 97 48.698 28.418 39.949 1.00 9.55 ATOM 713 O PHE A 97 49.054 27.761 38.962 1.00 9.51 ATOM 713 O PHE A 97 49.054 27.761 38.962 1.00 9.51 ATOM 715 CA ARG A 98 49.498 29.260 40.597 1.00 8.26 ATOM 716 CB ARG A 98 50.900 29.457 40.205 1.00 11.26 ATOM 717 CG ARG A 98 51.149 30.927 39.808 1.00 13.41 ATOM 718 CD ARG A 98 52.624 31.218 39.452 1.00 12.41 ATOM 719 NE ARG A 98 52.902 32.648 39.002 1.00 15.00 ATOM 719 NE ARG A 98 52.303 32.811 38.9670 1.00 19.61 ATOM 720 CZ ARG A 98 54.350 32.871 38.99.70 1.00 20.95 ATOM 721 NH1 ARG A 98 54.350 32.871 38.99.70 1.00 20.95 ATOM 722 NH2 ARG A 98 51.765 29.079 41.417 1.00 19.61 ATOM 723 C ARG A 98 51.765 29.079 41.417 1.00 19.61 ATOM 724 O ARG A 98 51.765 29.079 41.417 1.00 19.81 ATOM 725 N LYS A 99 52.258 29.881 42.327 1.00 12.72 ATOM 726 CA LYS A 99 52.179 26.922 43.688 1.00 10.488 ATOM 727 CB LYS A 99 53.744 27.518 42.557 1.00 10.80 ATOM 728 CG LYS A 99 53.744 27.518 45.557 1.00 10.62 ATOM 730 CE LYS A 99 53.809 26.095 41.956 1.00 13.56 ATOM 731 NZ LYS A 99 53.809 26.095 41.956 1.00 13.56 ATOM 732 C LYS A 99 53.809 26.095 41.956 1.00 14.42 ATOM 734 N ALA A 100 55.960 23.900 42.072 1.00 12.67 ATOM 735 CA ALA A 100 55.960 23.900 42.072 1.00 12.67 ATOM 736 CB ALA A 100 55.960 23.900 42.072 1.00 12.67 ATOM 737 C ALA A 100 55.960 23.900 42.072 1.00 14.42 ATOM 737 C ALA A 100 55.960 23.900 42.072 1.00 14.42 ATOM 738 O ALA A 100 55.960 23.900 42.072 1.00 13.81 ATOM 740 CA GLY A 101 56.631 19.274 41.195 1.00 13.56 ATOM 741 C GLY A 101 56.641 19.544 19.555 1.00 19.32 ATOM 742 C GLY A 101 56.664 19.545 10.00 13.81										A
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ATOM 718 CG ARG A 98 52.02 31.218 39.452 1.00 12.41 ATOM 718 CD ARG A 98 52.902 32.648 39.002 1.00 15.00 ATOM 719 NE ARG A 98 54.350 32.871 38.907 1.00 20.95 ATOM 720 CZ ARG A 98 54.350 32.871 38.907 1.00 20.95 ATOM 721 NH1 ARG A 98 54.454 34.446 40.606 1.00 16.05 ATOM 722 NH2 ARG A 98 55.048 33.714 39.670 1.00 19.61 ATOM 722 NH2 ARG A 98 56.361 33.824 39.500 1.00 22.95 ATOM 723 C ARG A 98 51.765 29.079 41.415 1.00 9.82 ATOM 724 O ARG A 98 51.765 29.079 41.415 1.00 9.82 ATOM 725 N LYS A 99 52.258 27.838 41.417 1.00 13.72 ATOM 726 CA LYS A 99 52.258 27.838 41.417 1.00 13.72 ATOM 726 CA LYS A 99 52.899 26.401 44.919 1.00 13.72 ATOM 728 CG LYS A 99 52.899 26.401 44.919 1.00 8.32 ATOM 729 CD LYS A 99 53.744 27.518 45.557 1.00 10.62 ATOM 730 CE LYS A 99 54.525 27.007 46.790 1.00 10.76 ATOM 731 NZ LYS A 99 55.346 28.125 47.368 1.00 13.56 ATOM 732 C LYS A 99 55.346 28.125 47.368 1.00 13.56 ATOM 733 O LYS A 99 53.809 26.095 41.956 1.00 14.43 ATOM 733 O LYS A 99 53.809 26.095 41.956 1.00 14.43 ATOM 733 NZ LYS A 99 53.200 25.056 41.701 1.00 15.34 ATOM 733 NZ LYS A 99 53.200 25.056 41.701 1.00 15.34 ATOM 733 NZ LYS A 99 53.200 25.056 41.701 1.00 15.34 ATOM 735 CA ALA A 100 55.912 26.226 41.769 1.00 12.67 ATOM 736 CB ALA A 100 55.912 26.226 41.769 1.00 14.43 ATOM 737 C ALA A 100 55.929 23.987 43.303 1.00 16.53 ATOM 738 O ALA A 100 55.929 23.987 43.303 1.00 16.53 ATOM 739 N GLY A 101 56.061 22.751 41.409 1.00 14.12 ATOM 744 C GGLY A 101 56.061 22.751 41.409 1.00 10.16 ATOM 744 C GGLY A 101 56.543 19.274 41.195 1.00 13.81 ATOM 744 C GGLY A 101 56.543 19.274 41.195 1.00 13.81 ATOM 745 C GLY A 102 56.273 18.156 40.313 1.00 16.58 ATOM 745 C GLY A 102 56.273 18.156 40.313 1.00 16.58 ATOM 747 N ASN A 103 54.624 17.451 41.976 1.00 17.72 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 749 CB ASN A 103 53.372 16.694 43.965 1.00 19.32	MOT	715	CA	ARG A	98	50.900	29.457	40.205	1.00 11.26	A
ATOM 718 CD ARG A 98 52.902 32.648 39.002 1.00 15.00 ATOM 719 NE ARG A 98 54.350 32.871 38.907 1.00 20.95 ATOM 720 CZ ARG A 98 55.048 33.714 39.670 1.00 19.61 ATOM 721 NH1 ARG A 98 55.048 33.714 39.670 1.00 19.61 ATOM 722 NH2 ARG A 98 56.361 33.824 39.500 1.00 22.95 ATOM 723 C ARG A 98 56.361 33.824 39.500 1.00 22.95 ATOM 723 C ARG A 98 51.765 29.079 41.415 1.00 9.82 ATOM 724 O ARG A 98 51.765 29.079 41.415 1.00 12.72 ATOM 725 N LYS A 99 52.258 27.838 42.327 1.00 12.72 ATOM 726 CA LYS A 99 52.258 27.838 41.417 1.00 13.72 ATOM 726 CA LYS A 99 52.258 27.838 41.417 1.00 13.72 ATOM 727 CB LYS A 99 52.899 26.401 44.919 1.00 8.32 ATOM 729 CD LYS A 99 52.899 26.401 44.919 1.00 8.32 ATOM 729 CD LYS A 99 53.744 27.518 45.557 1.00 10.62 ATOM 730 CE LYS A 99 53.744 27.518 45.557 1.00 10.62 ATOM 731 NZ LYS A 99 53.809 26.095 41.966 1.00 13.56 ATOM 732 C LYS A 99 53.809 26.095 41.966 1.00 13.56 ATOM 733 O LYS A 99 53.809 26.095 41.966 1.00 13.56 ATOM 733 O LYS A 99 53.200 25.056 41.701 1.00 15.34 ATOM 736 CB ALA A 100 55.120 26.226 41.769 1.00 14.53 ATOM 736 CB ALA A 100 55.910 25.056 41.701 1.00 14.53 ATOM 737 C ALA A 100 55.929 23.987 43.303 1.00 16.53 ATOM 739 N GLY A 101 56.061 22.751 41.409 1.00 14.53 ATOM 739 N GLY A 101 56.061 22.751 41.409 1.00 10.16 ATOM 741 C GLY A 101 56.061 22.751 41.409 1.00 11.78 ATOM 742 C GLY A 101 56.061 22.751 41.409 1.00 10.16 ATOM 744 CA GLY A 101 56.54 19.274 41.195 1.00 13.81 ATOM 744 CA GLY A 101 56.54 19.274 41.195 1.00 13.81 ATOM 745 C GLY A 101 56.54 19.275 41.98 10.0 13.81 ATOM 745 C GLY A 101 56.54 19.275 42.98 1.00 16.54 ATOM 747 N ASN A 103 55.269 41.741 1.976 1.00 16.54 ATOM 747 N ASN A 103 54.624 17.451 41.976 1.00 16.54 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.58 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.58 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.93 1.00 16.54 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.93 1.00 16.93 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.93 1.00 19.32	MOTA	716	CB	ARG A	98	51.149	30.927	39.808	1.00 13.41	A
ATOM 718 CD ARG A 98 52.902 32.648 39.002 1.00 15.00 ATOM 719 NE ARG A 98 54.350 32.871 38.907 1.00 20.95 ATOM 720 CZ ARG A 98 55.048 33.714 39.670 1.00 19.61 ATOM 721 NH1 ARG A 98 55.048 33.714 39.670 1.00 19.61 ATOM 722 NH2 ARG A 98 56.361 33.824 40.606 1.00 16.05 ATOM 722 NH2 ARG A 98 56.361 33.824 39.500 1.00 22.95 ATOM 723 C ARG A 98 51.765 29.079 41.415 1.00 9.82 ATOM 724 O ARG A 98 51.765 29.079 41.415 1.00 12.72 ATOM 725 N LYS A 99 52.258 27.838 41.417 1.00 13.72 ATOM 726 CA LYS A 99 52.258 27.838 41.417 1.00 13.72 ATOM 726 CA LYS A 99 52.258 27.838 41.417 1.00 14.88 ATOM 727 CB LYS A 99 52.899 26.401 44.919 1.00 8.32 ATOM 729 CD LYS A 99 52.899 26.401 44.919 1.00 8.32 ATOM 729 CD LYS A 99 53.744 27.518 45.557 1.00 10.62 ATOM 730 CE LYS A 99 53.744 27.518 45.557 1.00 10.62 ATOM 731 NZ LYS A 99 53.809 26.095 41.766 1.00 14.43 ATOM 732 C LYS A 99 53.809 26.095 41.766 1.00 14.43 ATOM 733 O LYS A 99 53.809 26.095 41.769 1.00 12.67 ATOM 735 CA ALA A 100 55.120 26.226 41.769 1.00 12.67 ATOM 736 CB ALA A 100 55.910 25.056 41.701 1.00 14.53 ATOM 737 C ALA A 100 55.929 23.987 43.303 1.00 14.53 ATOM 738 O ALA A 100 55.929 23.987 43.303 1.00 16.53 ATOM 739 N GLY A 101 56.061 22.751 41.409 1.00 11.78 ATOM 741 C GLY A 101 56.061 22.751 41.409 1.00 10.16 ATOM 742 C GLY A 101 56.061 22.751 41.409 1.00 11.78 ATOM 742 C GLY A 101 56.061 22.751 41.409 1.00 11.78 ATOM 742 C GLY A 101 56.54 19.275 41.956 1.00 14.78 ATOM 744 CA GLY A 101 56.54 19.275 41.956 1.00 17.78 ATOM 745 C GLY A 101 56.54 19.275 41.956 1.00 17.78 ATOM 745 C GLY A 102 56.273 18.156 40.313 1.00 20.81 ATOM 745 C GLY A 102 56.273 18.156 40.313 1.00 16.54 ATOM 745 C GLY A 102 56.273 18.156 40.313 1.00 16.54 ATOM 747 N ASN A 103 54.624 17.451 41.976 1.00 16.54 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.58 ATOM 749 CB ASN A 103 53.465 15.760 44.615 1.00 23.02 ATOM 749 CB ASN A 103 54.624 17.451 41.976 1.00 16.93 100 16.58 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 749 CB ASN A 103 53.465 15.760 44.615 1.00 23.02	MOT	717	CG	ARG A	98	52.624	31.218	39.452	1.00 12.41	А
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ATOM 739 N GLY A 101 56.061 22.751 41.409 1.00 10.16 ATOM 740 CA GLY A 101 56.133 21.476 42.096 1.00 11.78 ATOM 741 C GLY A 101 55.786 20.360 41.136 1.00 17.78 ATOM 742 O GLY A 101 55.853 20.479 40.338 1.00 14.78 ATOM 743 N GLY A 102 56.543 19.274 41.195 1.00 13.81 ATOM 744 CA GLY A 102 56.573 18.156 40.313 1.00 20.81 ATOM 745 C GLY A 102 55.051 17.348 40.720 1.00 16.58 ATOM 746 O GLY A 102 55.051 17.348 40.720 1.00 16.58 ATOM 747 N ASN A 103 54.624 17.451 41.976 1.00 17.72 ATOM 748 CA ASN A 103 53.465 16.675 42.434 1.00 16.85 ATOM 749 CB ASN A 103 53.372 16.694 43.963 1.00 15.22 ATOM 750 CG ASN A 103 54.365 15.760 44.615 1.00 23.02 ATOM 751 OD1 ASN A 103 55.279 15.249 43.955 1.00 19.32	TOM	73B	0	ALA A	100					A
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ATOM 752 ND2 ASN A 103 54.205 15.535 45.916 1.00 15.75									1.00 15.75	A
ATOM 753 C ASN A 103 52.145 17.197 41.885 1.00 15.38									1.00 15.38	A
ATOM 754 O ASN A 103 51.991 18.390 41.666 1.00 11.02		754	0	ASN A	103		18.390			A
ATOM 755 N ALA A 104 51.183 16.306 41.693 1.00 16.02		755	N	ALA A	104	51.183	16.306			A

ATOM	756	CA	ALA A 104	49.880	16 744	41 210	1 00 16 65	_
ATOM	757	CB	ALA A 104		16.744	41.219	1.00 16.65	A
ATOM	758	C	ALA A 104	49.068	15.538	40.741	1.00 20.27	A
ATOM	759	ŏ		49.170	17.427	42.395	1.00 15.98	A
ATOM			ALA A 104	49.298	16.986	43.531	1.00 15.25	A
	760	N	VAL A 105	48.470	18.530	42.127	1.00 13.62	A
ATOM	761	CA	VAL A 105	47.701	19.227	43.157	1.00 13.77	A
ATOM	762	CB	VAL A 105	47.708	20.756	42.945	1.00 15.80	A
MOTA	763	CG1	VAL A 105	46.645	21.409	43.814	1.00 16.24	Ä
MOTA	764	CG2		49.081	21.310	43.295	1.00 15.48	Ä
MOTA	765	С	VAL A 105	46.273	18.699	43.026	1.00 13.40	Ä
MOTA	766	0	VAL A 105	45.634	18.867	41.982		
ATOM	767	N	ASP A 106	45.781	18.059			A
MOTA	768	CA	ASP A 106			44.085	1.00 11.30	A
MOTA	. 769	CB	ASP A 106	44.446	17.447	44.087	1.00 13.33	A
ATOM	770	CG	700 X 100	44.594	15.914	44.007	1.00 15.23	A
ATOM	771	OD1	ASP A 106 ASP A 106	43.266	15.181	43.763	1.00 18.75	A
ATOM	772	OD2		43.294	13.932	43.636	1.00 20.08	A
ATOM	773			42.201	15.832	43.705	1.00 16.37	A
	_	C	ASP A 106	43.748	17.854	45.371	1.00 13.44	A
ATOM	774	0	ASP A 106	44.013	17.312	46.441	1.00 12.47	. A
ATOM	775	N	LEU A 107	42.838	18.809	45.256	1.00 12.47	A
ATOM	776	CA	LEU A 107	42.126	19.322	46.424	1.00 10.60	A
ATOM	777	CB	LEU A 107	41.608	20.743	46.139	1.00 9.94	A
ATOM	778	CG	LEU A 107	42.656	21.830	45.874	1.00 15.11	A
ATOM	779	CD1	LEU A 107	41.992	23.049	45.233	1.00 12.77	A
ATOM	780	CD2	LEU A 107	43.332	22.222	47.191	1.00 15.50	Ä
ATOM	781	C	LEU A 107	40.936	18.504	46.860	1.00 11.58	A
ATOM	782	0	LEU A 107	40.118	18.134	46.029	1.00 11.26	
ATOM	783	N	SER A 108	40.840	18.205	48.157	1.00 10.03	A
ATOM	784	CA	SER A 108	39.632	17.555	48.632		A
ATOM	785	CB	SER A 108	39.823	16.938		1.00 9.49	Ā
ATOM	786	OG	SER A 108	40.112		50.026	1.00 11.45	Ā
ATOM	787	c	SER A 108		17.944	50.988	1.00 10.62	A
ATOM	788			38.686	18.762	48.734	1.00 13.88	A
ATOM		0	SER A 108	39.137	19.909	48.733	1.00 9.31	A
	789	N	VAL A 109	37.384	18.528	48.795	1.00 11.62	Α
ATOM	790	CA	VAL A 109	36.456	19.648	48.915	1.00 12.52	A
ATOM	791	CB	VAL A 109	34.997	19.149	48.822	1.00 14.25	Α
ATOM	792	CG1	VAL A 109	34.022	20.273	49.172	1.00 10.43	Α
ATOM	793	CG2	VAL A 109	34.738	18.624	47.385	1.00 9.95	A
ATOM	794	Ç	VAL A 109	36.705	20.397	50.228	1.00 8.60	A
ATOM	795	0	VAL A 109	36.646	21.622	50.265	1.00 9.21	A
ATOM	796	N	LYS A 110	36.995	19.666	51.301	1.00 9.28	A
ATOM	797	CA	LYS A 110	37.307	20.306	52.593	1.00 7.04	A
ATOM	798	CB	LYS A 110	37.597	19.237	53.650	1.00 7.60	A
ATOM	799	CG	LYS A 110	38.038	19.793	55.030	1.00 9.51	Ä
ATOM	800	CD	LYS A 110	36.987	20.726	55.655	1.00 7.71	A
ATOM	801	CE	LYS A 110	37.436	21.170	57.033	1.00 15.09	A
ATOM	802	NZ	LYS A 110	36.482	22.129	57.688	1.00 11.10	Ä
ATOM	803	С	LYS A 110	38.532	21.234	52.452	1.00 8.55	A
ATOM	804	0	LYS A 110	38.588	22.313	53.040	1.00 9.65	A
ATOM	805	N	GLU A 111	39.530	20.803	51.696	1.00 8.56	Ä
ATOM	806	CA	GLU A 111	40.711	21.640	51.495	1.00 11.39	Ā
ATOM	807	CB	GLU A 111	41.817	20.836	50.800	1.00 13.45	Ä
ATOM	808	CG	GLU A 111	42.582	19.940	51.784	1.00 15.25	Ä
ATOM	809	CD	GLU A 111	43.527	18.960	51.098	1.00 16.99	Ä
ATOM	810	OE1	GLU A 111	44.310	18.296	51.808		
ATOM	811	OE2	GLU A 111	43.477	18.851	49.860	1.00 12.70 1.00 13.80	A
ATOM	812	č	GLU A 111	40.342	22.881	50.663		A
ATOM	813	ŏ	GLU A 111	40.751	23.998	50.983	1.00 12.16	A
ATOM	814	Ŋ	LEU A 112	39.586			1.00 8.45	A
ATOM	815	CA	LEU A 112		22.680	49.587	1.00 11.50	A
ATOM	816			39.157	23.802	48.753	1.00 11.60	A
		CB	LEU A 112	38.127	23.339	47.728	1.00 12.29	A
ATOM	817	CG	LEU A 112	37.520	24.486	46.906	1.00 13.68	A
ATOM	818	CD1	LEU A 112	38.486	24.835	45.793	1.00 14.87	A
ATOM	819	CD2	LEU A 112	36.183	24.067	46.307	1.00 23.81	A
ATOM	820	C	LEU A 112	38.491	24.845	49.648	1.00 11.64	A
ATOM	821	0	LEU A 112	38.782	26.036	49.569	1.00 9.35	A
ATOM	822	N	CYS A 113	37.598	24.370	50.511	1.00 9.13	A
MOTA	823	CA	CYS A 113	36.869	25.251	51.407	1.00 10.02	A
MOTA	824	С	CYS A 113	37.806	26.040	52.332	1.00 10.42	A
ATOM	825	0	CYS A 113	37.620	27.243	52.550	1.00 9.94	A
ATOM ·	826	CB	CYS A 113	35.881	24.414	52.215	1.00 7.06	A
ATOM	827	SG	CYS A 113	34.495	23.714	51.225	1.00 12.97	A
ATOM	828	N	GLY A 114	38.815	25.357	52.854	1.00 8.53	Ä
ATOM	829	CA	GLY A 114	39.774	25.979	53.746	1.00 8.15	À
ATOM	830	C	GLY A 114	40.615	27.023	53.048	1.00 8.58	Ä
ATOM	831	ŏ	GLY A 114	40.974	28.045	53.660	1.00 9.42	Ä
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ATOM	832	N	VAL A	115	40.929	26.780	51.773	1.00	8.91	Α
ATOM	833	CA	VAL A	115	41.724	27.727	51.001	1.00 1		Ä
ATOM	834	CB	VAL A	115	42.142	27.154	49.611		.0.97	
ATOM	835	CG1	VAL A		42.754	28.274	48.736			A
ATOM	836	CG2	VAL A		43.175	26.034	49.794		.2.08	A
ATOM	837	c	VAL A					1.00	9.96	A
ATOM	838	ŏ			40.933	28.999	50.769		.0.50	Α
	839		VAL A		41.450	30.107	50.958		.0.53	Α
ATOM		N	PHE A		39.672	28.856	50.383	1.00 1	.0.04	A
ATOM	840	CA	PHE A		38.885	30.046	50.123	1.00 1	.2.53	A
ATOM	841	CB	PHE A	116	37.891	29.774	49.000	1.00	8.51	Α
ATOM	842	CG	PHE A		38.564	29.656	47.664	1.00	8.77	A
ATOM	843	CD1	PHE A	116	39.041	28.429	47.220	1.00	7.52	A
MOTA	844	CD2	PHE A	116	38.792	30.791	46.892	1.00 1		Ä
ATOM	845	CE1	PHE A		39.742	28.319	46.019		1.26	
ATOM	846	CE2	PHE A		39.494	30.708	45.682			A
MOTA	847	CZ	PHE A		39.971	29.463			2.98	A
ATOM	848	č	PHE A		38.236	30.713	45.244	1.00 1		A
ATOM	849	ŏ	PHE A				51.319		1.72	A
ATOM	850	Ŋ			37.688	31.802	51.180		0.01	A
ATOM			SER A		38.323	30.077	52.493	1.00	7.36	Α
	851	CA	SER A		37.802	30.669	53.722	1.00 1	2.12	Α
ATOM	852	CB	SER A		37.217	29.605	54.654	1.00 1	1.41	A
ATOM	853	ОĞ	SER A		38.251	28.827	55.231	1.00 1	2.73	A
MOTA	854	C	SER A		38.935	31.372	54.474	1.00 1	2.93	A
MOTA	855	0	SER A		38.693	32.241	55.316	1.00	9.90	Α
ATOM	856	N	GLY A	. 118	40.169	30.988	54.174	1.00 1		A
MOTA	857	CA	GLY A	118	41.312	31.576	54.860		3.07	A
ATOM	858	C	GLY A	118	41.850	30.640	55.931	–	5.32	A
ATOM	859	0	GLY A		42.935	30.873	56.484		5.65	A
ATOM	860	N	ARG A		41.107	29.575	56.241	1.00 1		
ATOM	861	CA	ARG A		41.550	28.622	57.266	1.00 1		A
ATOM	862	CB	ARG A		40.503	27.518	57.485			A
MOTA	863	ĊĠ	ARG A		40.986	26.359		1.00 1		Ā
ATOM	864	CD					58.390	1.00 1		Ą
ATOM			ARG A		39.880	25.325	58.628	1.00 1		A
	865	NE	ARG A		39.338	24.771	57.377	1.00 1		A
ATOM	866	CZ	ARG A		39.828	23.717	56.727	1.00 1	3.77	A
ATOM	867	NH1	ARG A		40.895	23.061	57.188	1.00	9.19	Α
ATOM	868		ARG A		39.239	23.317	55.607	1.00 1	0.56	Α
MOTA	869	С	ARG A		42.896	27.990	56.896	1.00 1	4.09	Α
MOTA	870	0	ARG A	. 119	43.749	27.784	57.757	1.00 1	2.49	Α
ATOM	871	N	ILE A	120	43.074	27.672	55.620		4.25	A
ATOM	872	CA	ILE A	120	44.327	27.088	55.134		1.87	Ä
ATOM	873	CB	ILE A	120	44.066	25.956	54.113	1.00 1		A
ATOM	874	CG2	ILE A		45.373	25.443	53.529		2.88	Â
ATOM	875	CG1	ILE A		43.349	24.796	54.812	1.00 1		Ä
ATOM	876	CDI	ILE A		42.920	23.638	53.863		2.93	
ATOM	877	Č	ILE A		45.042	28.241				A
ATOM	878	ŏ	ILE A		44.606	28.704	54.445		6.50	A
ATOM	879	Ŋ	ALA A				53.391	1.00 1		A
ATOM	880	CA	ALA A		46.131	28.706	55.051		5.30	A
					46.884	29.848	54.529		4.70	A
ATOM	881	CB	ALA A		47.111	30.850	55.640		1.39	A
ATOM	882	Č	ALA A		48.211	29.482	53.904		5.45	A
ATOM	883	0	ALA A		48.868	30.329	53.284		б.44	A
ATOM	884	N	ASN A		48.608	28.227	54.056		2.07	A
ATOM	885	CA	ASN A		49.887	27.789	53.507	1.00 1		A
ATOM	886	CB	ASN A		50.853	27.467	54.660	1.00 1		Α
ATOM	887	CG	ASN A		52.279	27.293	54.188	1.00 1	6.68	Α
ATOM	888	OD1	ASN A	122	52.666	26.224	53.725	1.00 1	8.01	A
MOTA	889	ND2	ASN A	122	53.063	28.363	54.279	1.00 1	4.68	Α
MOTA	890	С	ASN A		49.681	26.568	52.608	1.00 1		A
ATOM	891	0	ASN A	122	48.809	25.737	52.865	1.00 1		Α
ATOM	892	N	TRP A	123	50.454	26.499	51.528	1.00 1		A
ATOM	893	CA	TRP A	123	50.365	25.390	50.580	1.00 1		A
ATOM	894	CB		123	51.330	25.597	49.406	1.00 1		Ä
ATOM	895	CG	TRP A	123	50.761	26.503	48.337	1.00 1		Ä
ATOM	896		TRP A	123	49.900	26.108	47.261	1.00 1		
ATOM	897	CE2	TRP A			27.279				A
ATOM	898	CE3			49.568 49.381		46.533		2.26	A
			TRP A			24.884	46.841	1.00 1		A
ATOM	899		TRP A		50.916	27.862	48.227		5.24	A
ATOM	900	NE1		123	50.198	28.334	47.140		2.70	A
ATOM	901	CZ2	TRP A		48.732	27.256	45.403	1.00 1		A
ATOM	902	CZ3	TRP A		48.547	24.863	45.710		6.36	A
ATOM	903	CH2		123	48.237	26.043	45.012		9.72	A
ATOM	904	Č	TRP A		50.661	24.045	51.213		3.55	A
ATOM	905	0	TRP A		50.284	23.006	50.676	1.00 1	3.98	A
MOTA	906	N	SER A		51.346	24.054	52.349	1.00 1	3.10	Α
ATOM	907	CA	SER A	124	51.654	22.801	53.010	1.00 1	1.36	A

ATOM	908	СВ	SER A	124	52.670	23.038	54.135	1.00 1	1.89	A
ATOM	909	OG	SER A	124	52.130	23.884	55.132	1.00 1		A
MOTA	910	C	SER A		50.361	22.161	53.564	1.00 1		. A
ATOM ATOM	911 912	O N	SER A GLY A		50.354 49.273	20.974 22.937	53.924 53.617		.3.81 .3.73	A A
ATOM	913	CA	GLY A		47.999	22.416	54.117	1.00 1		A
MOTA	914	Ç	GLY A	125	47.216	21.569	53.101		9.05	A
ATOM	915	O.	GLY A		46.116	21.066	53.404		5.82	A
ATOM ATOM	916 917	N CA	ILE A		47.759 47.111	21.413 20.590	51.892 50.866	1.00 1	.3.57	A A
ATOM	918	СВ	ILE A		47.116	21.338	49.499		0.65	A
MOTA	919	CG2	ILE A		46.584	20.440	48.369		0.73	A
ATOM	920	CG1	ILE A		46.244	22.598	49.639		4.04	A
ATOM ATOM	921 922	CD1 C	ILE A		46.355 47.886	23.571 19.270	48.474 50.794	1.00 2	21.47	A A
ATOM	923	ŏ	ILE A		49.012	19.228	50.299		2.48	A
ATOM	924	N	THR A		47.287	18.199	51.310		4.33	A
MOTA MOTA	925 926	CA CB	THR A		47.974 47.144	16.918 15.848	51.341 52.079	1.00 1		A A
ATOM	927	OG1	THR A		45.978	15.519	51.309		1.71	Ä
ATOM	928	CG2	THR A	127	46.719	16.379	53.462	1.00 1		A
ATOM	929	C	THR A		48.389	16.389	49.978		15.85	A
ATOM ATOM	930 931	O N	THR A		47.628 49.627	16.442 15.907	49.011 49.925	1.00 1	L5.48 L1.25	A A
ATOM	932	CA	GLY A		50.202	15.348	48.719		3.92	A
ATOM	933	C	GLY A		50.726	16.299	47.655		15.93	A
ATOM ATOM	934 935	O N	GLY A ALA A		51.360 50.491	15.837 17.610	46.718 47.788	1.00 1	L8.28 L3.36	A A
ATOM	936	CA	ALA A			18.558	46.765		14.53	A
ATOM	937	CB	ALA A		50.138	19.873	46.886	1.00 1	13.51	Α
ATOM	938	C	ALA A		52.428	18.856 19.427	46.777		20.08 L3.92	A
ATOM ATOM	939 940	N O	ALA A GLY A		52.954 53.110	18.489	45.811 47.863		15.72	A A
ATOM	941	CA	GLY A	130	54.552	18.715	47.931	1.00 1	18.22	A
ATOM	942	Č	GLY A		54.937	20.167	47.720		17.01	A
ATOM ATOM	943 944	O N	GLY A ARG A		55.944 54.130	20.485 21.059	47.088 48.274	1.00 1	LG.95 L4.88	A A
ATOM	945	CA	ARG A		54.361	22.500	48.142		4.67	Ä
MOTA	946	CB	ARG A		53.312	23.102	47.190		10.65	A
ATOM ATOM	947 948	CG CD	ARG A		53.506 52.234	22.713 22.985	45.730 44.895		L4.78 L3.27	A A
ATOM	949	NE	ARG A		52.479	22.959	43.441	1.00		A
ATOM	950	CZ	ARG A		52.670	21.873	42.695		12.12	A
ATOM ATOM	951 952	NH1 NH2	ARG A		52.880 52.656	22.010 20.660	41.383		L2.83 L3.76	A A
ATOM	953	C	ARG A		54.217	23.171	49.502		L4.12	Ä
ATOM	954	0	ARG A	131	53.451	22.703	50.329	1.00	L5.12	A
ATOM	955	N	SER A		54.948	24.258	49.730		12.39	A A
ATOM ATOM	956 957	CA CB	SER A		54.830 55.817	24.987 24.450	50.990 52.046		15.94 22.25	A
ATOM	958	ŌĠ	SER A		57.143	24.690	51.644	1.00 2	25.99	A
ATOM	959	Č	SER A		55.070	26.468	50.735		12.92	A
ATOM ATOM	960 961	O N	SER A GLY A		55.695 54.570	26.857 27.300	49.746 51.634		L6.84 L4.33	A A
ATOM	962	CA	GLY A		54.695	28.734	51.442	1.00	14.73	· A
ATOM	963	Ç	GLY A		53.295	29.318	51.394	1.00 1		A
ATOM ATOM	964 965	O N	GLY A PRO A	133	52.320 53.162	28.589 30.633	51.183 51.561	1.00		A A
ATOM	966	CD	PRO A		54.254	31.607	51.743	1.00		A
ATOM	967	CA	PRO A		51.854	31.291	51.548	1.00		A
ATOM ATOM	968 969	CB CG	PRO A		52.196 53.623	32.760 32.900	51.828 51.266	1.00 2		A A
ATOM	970	č	PRO A		50.997	31.143	50.299	1.00	16.29	A
ATOM	971	0	PRO A		51.509	31.105	49.180	1.00		A
ATOM ATOM	972 973	N CA	ILE A		49.685 48.688	31.057 30.973	50.527 49.454	1.00		A A
ATOM	974	CB	ILE A		47.523	30.010	49.801	1.00	15.95	Ä
MOTA	975	CG2	ILE A	135	46.417	30.115	48.727	1.00		A
ATOM	976 977	CG1 CD1	ILE A		48.032 46.988	28.582 27.607	49.918 50.453	1.00	15.73 15.61	A A
ATOM ATOM	977 978	CDI	ILE A		48.077	32.366	49.353	1.00		Ä
ATOM	979	0	ILE A	135	47.757	32.983	50.372	1.00		A
ATOM	980 981	N CA	GLN A		47.918 47.319	32.872 34.190	48.136 47.958	1.00		A A
ATOM ATOM	982	CB	GLN A		48.317	35.145	47.306	1.00		Ä
ATOM	983	CG	GLN A		47.892	36.594	47.337	1.00	19.42	A

ATOM ATOM	984 985	CD OE1		A 136 A 136	48.999		46.905	1.00 23.10	Α
MOTA	986	NE2	GLN	A 136	49.620 49.233	37.403 38.585	45.858 47.714	1.00 23.52 1.00 30.84	A A
ATOM ATOM	987 988	C O		A 136 A 136	46.105	34.023	47.053	1.00 9.51	Ä
ATOM	989	N		A 137	46.254 44.911	33.639 34.303	45.921 47.552	1.00 9.81 1.00 8.18	A A
ATOM ATOM	990 991	CA CB		A 137	43.717	34.161	46.733	1.00 4.96	A
ATOM	992	CG1	VAL	A 137 A 137	42.470 41.176	33.907 34.014	47.657 46.855	1.00 8.36	A
ATOM ATOM	993	CG2	VAL .	A 137	42.589	32.543	48.294	1.00 5.20 1.00 10.61	A A
ATOM	994 995	C		A 137 A 137	43.442 43.555	35.380 36.534	45.837 46.284	1.00 9.91	A
ATOM ATOM	996	N	VAL,	A 138	43.124	35.114	44.566	1.00 9.14 1.00 7.01	A A
ATOM	997 998	CA CB		A 138 A 138	42.735 43.437	36.134 35.976	43.600 42.226	1.00 8.67 1.00 9.91	A
ATOM ATOM	999 1000	CG1	VAL	A 138	42.983	37.092	41.301	1.00 9.91 1.00 11.71	A A
MOTA	1001	CG2 C		A 138 A 138	44.947 41.237	36.068 35.914	42.394 43.386	1.00 18.67 1.00 7.40	A A
ATOM ATOM	1002 1003	O N	VAL A	A 138	40.791	34.775	43.196	1.00 7.75	A
ATOM	1003	CA	TYR A	A 139 A 139	40.452 39.009	36.987 36.871	43.435 43.256	1.00 9.87 1.00 9.42	A A
MOTA MOTA	1005 1006	CB CG		A 139	38.303	36.902	44.625	1.00 8.26	A
MOTA	1007	CD1	TYR A	A 139 A 139	38.509 37.570	38.192 39.211	45.389 45.322	1.00 9.37 1.00 8.61	A A
MOTA MOTA	1008 1009	CE1 CD2	TYR A		37.748	40.424	46.013	1.00 9.72	Ä
MOTA	1010	CE2	TYR A	A 139	39.659 39.853	38.397 39.616	46.177 46.878	1.00 9.71 1.00 12.90	A A
ATOM ATOM	1011 1012	CZ OH	TYR A	A 139	38.890 39.045	40.623	46.786	1.00 15.66	. A
MOTA	1013	С	TYR A	A 139	38.507	41.829 38.006	47.459 42.381	1.00 8.23 1.00 8.45	A A
ATOM ATOM	1014 1015	O N	TYR A		39.246 37.259	38.947	42.099	1.00 8.15	A
MOTA	1016	CA	ARG A	140	36.660	37.899 38.903	41.935 41.070	1.00 8.93 1.00 7.41	A A
ATOM ATOM	1017 1018	CB CG	ARG A		35.514 35.991	38.296 37.317	40.243 39.148	1.00 10.32	A
ATOM	1019	CD	ARG A	140	36.556	38.103	37.948	1.00 5.86 1.00 5.80	A A
ATOM ATOM	1020 1021	NE CZ	ARG A		35.502 34.659	38.821 38.232	37.218 36.376	1.00 7.23 1.00 11.87	A
MOTA MOTA	1022	NH1	ARG A	140	34.748	36.918	36.152	1.00 11.87 1.00 5.93	A A
MOTA	1023 1024	NH2 C	ARG A		33.715 36.129	38.952 40.063	35.769 41.895	1.00 8.31 1.00 8.44	A A
ATOM ATOM	1025 1026	0 N	ARG A		35.327	39.896	42.832	1.00 8.91	Ä
ATOM	1027	CA	ALA A		36.583 36.198	41.242 42.471	41.523 42.206	1.00 8.44 1.00 8.99	A A
ATOM ATOM	1028 1029	CB C	ALA A		37.121	43.579	41.761	1.00 12.40	A
MOTA	1030	ŏ	ALA A		34.748 34.091	42.895 43.421	41.975 42.878	1.00 11.15 1.00 9.17	A A
ATOM ATOM	1031 1032	N CA	GLU A		34.258 32.912	42.679 43.110	40.765	1.00 10.41	A
MOTA	1033	CB	GLU A	142	32.944	43.735	40.401 38.995	1.00 11.28 1.00 11.17	A A
ATOM ATOM	1034 1035	CG CD	GLU A		32.968 34.319	42.720 41.984	37.800 37.551	1.00 16.02 1.00 14.71	A
MOTA	1036	OE1	GLU A	142	35.102	41.758	38.492	1.00 14.71	A A
ATOM ATOM	1037 1038	OE2 C	GLU A		34.582 31.854	41.608 42.001	36.382 40.428	1.00 15.07 1.00 15.45	A A
ATOM ATOM	1039 1040	0	GLU A		32.160	40.827	40.689	1.00 11.17	Â
MOTA	1041	N CA	VAL A		30.604 29.474	42.399 41.461	40.170 40.114	1.00 13.82 1.00 12.65	A A
ATOM ATOM	1042 1043	CB CG1	VAL A		28.155	42.192	39.792	1.00 12.26	A
MOTA	1044	CG2	VAL A	143	27.052 27.822	41.196 43.174	39.668 40.870	1.00 17.81 1.00 18.80	A A
ATOM ATOM	1045 1046	C	VAL A		29.770 29.785	40.456 40.814	38.996	1.00 12.06	A
ATOM	1047	N	SER A	144	29.972	39.198	37.811 39.388	1.00 10.75 1.00 10.21	A A
ATOM ATOM	1048 1049	CA CB	SER A		30.352 31.822	38.119 37.764	38.462 38.758	1.00 6.60	A
ATOM	1050	QG	SER A	144	32.188	36.468	38.328	1.00 8.21 1.00 8.64	A A
ATOM ATOM	1051 1052	C	SER A		29.499 29.166	36.834 36.346	38.512 39.601	1.00 7.57 1.00 8.05	A
MOTA	1053	N	GLY A	145	29.168	36.303	37.330	1.00 5.34	A A
ATOM ATOM	1054 1055	CA C	GLY A GLY A		28.437 29.335	35.047 33.884	37.226 37.638	1.00 7.72 1.00 7.84	A A
ATOM	1056	0	GLY A	145	28.873	32.870	38.197	1.00 6.69	A
ATOM ATOM	1057 1058	N CA	THR A		30.628 31.574	34.001 32.953	37.357 37.758	1.00 6.57 1.00 6.39	A A
MOTA	1059	CB	THR A		33.012	33.263	37.279	1.00 9.37	A

ATOM	1060	OG1	THO R		22 22				
ATOM	1061	CG2	THR A	1 146	33.026	33.463	35.855	1.00 8.49	A
ATOM	1062			1 146	33.928	32.087	37.613	1.00 11.25	A
ATOM		C	THR A		31.569	32.892	39.294	1.00 8.02	A
	1063	Ö.	THR A		31.601	31.802	39.888	1.00 8.00	A
ATOM	1064	N	THR A		31.551	34.064	39.930	1.00 6.33	A
ATOM	1065	CA	THR A		31.483	34.131	41.394	1.00 8.35	A
MOTA	1066	CB	THR A	147	31.554	35.591	41.921	1.00 6.29	Ä
ATOM	1067	OG1	THR A	147	32.834	36.161	41.624	1.00 7.92	Ä
MOTA	1068	CG2	THR A	147	31.373	35.602	43.450	1.00 8.46	Ä
ATOM	1069	C	THR A		30.175	33.486	41.885	1.00 5.86	
ATOM	1070	0	THR A		30.172	32.745	42.883		A
ATOM	1071	N	GLU A		29.059	33.751	41.198	1.00 7.90 1.00 5.81	A
ATOM	1072	CA	GLU A		27.786	33.131	41.592	_ ::	Ā
ATOM	1073	CB	GLU A		26.644	33.653		1.00 5.50	A
ATOM	1074	ČĞ	GLU A		25.284		40.710	1.00 6.06	A
ATOM	1075	CD	GLU A		24.076	33.004	41.058	1.00 10.99	A
ATOM	1076	OE1				33.737	40.457	1.00 12.04	A
ATOM	1077	OE2			23.920	34.966	40.685	1.00 9.92	A
ATOM	1078				23.271	33.078	39.765	1.00 13.03	A
ATOM		C	GLU A		27.846	31.591	41.491	1.00 6.20	Α
	1079	O	GLU A		27.419	30.866	42.408	1.00 7.44	A
ATOM	1080	N	LEU A		28.318	31.077	40.359	1.00 4.66	A
ATOM	1081	CA	LEU A		28.442	29.616	40.196	1.00 6.87	Α
ATOM	1082	CB	LEU A		29.011	29.301	38.807	1.00 7.74	A
ATOM	1083	CG	LEU A		28.105	29.569	37.591	1.00 8.75	A
MOTA	1084		LEU A		28.878	29.218	36.342	1.00 10.50	A
MOTA	1085		LEU A		26.804	28.721	37.678	1.00 9.52	A
ATOM	1086	C	LEU A	149	29.376	28.980	41.254	1.00 7.07	A
ATOM	1087	0	LEU A	149	29.127	27.865	41.754	1.00 7.65	Ä
ATOM	1088	N	PHE A	150	30.473	29.670	41.568	1.00 8.71	Ä
MOTA	1089	CA	PHE A	150	31.459	29.183	42.540	1.00 7.06	A
ATOM	1090	CB	PHE A	150	32.752	30.021	42.427	1.00 6.97	Ä
ATOM	1091	CG		150	33.884	29.551	43.325	1.00 9.24	
ATOM	1092			150	34.313	28.225	43.305	1.00 10.27	A
ATOM	1093	CD2		150	34.557	30.455	44.138		A
ATOM	1094	CE1	PHE A		35.411	27.803		1.00 12.03	Ā
ATOM	1095	CE2	PHE A		35.657		44.081	1.00 12.21	Ā
ATOM	1096	CZ	PHE A			30.050	44.920	1.00 11.31	Ā
ATOM	1097	Č	PHE A		36.083	28.721	44.890	1.00 10.56	Ā
ATOM	1098	ŏ	PHE A		30.936	29.217	43.987	1.00 7.58	A
ATOM					31.060	28.236	44.709	1.00 6.52	A
ATOM	1099	N	THR A		30.350	30.334	44.409	1.00 7.57	A
	1100	CA	THR A		29.836	30.437	45.770	1.00 8.97	A
ATOM	1101	CB	THR A		29.548	31.938	46.193	1.00 9.78	A
ATOM	1102	OG1	THR A		28.580	32.526	45.314	1.00 8.77	A
ATOM	1103	CG2	THR A		30.826	32.744	46.152	1.00 7.96	A
ATOM	1104	Ċ	THR A		28.588	29.588	45.988	1.00 7.22	Α
ATOM	1105	0	THR A		28.274	29.245	47.131	1.00 7.49	A
ATOM	1106	N	ARG A		27.873	29.229	44.916	1.00 5.13	A
ATOM	1107	CA	ARG A	152	26.715	28.351	45.099	1.00 9.17	A
ATOM ·	1108	CB	ARG A	152	25.914	28.189	43.796	1.00 9.15	A
ATOM	1109	CG	ARG A	152	24.606	27.376	43.974	1.00 10.79	A
ATOM	1110	CD	ARG A	152	23.671	27.529	42.755	1.00 17.61	A
MOTA	1111	NE	ARG A	152	23.071	28.868	42.641	1.00 14.93	Ā
ATOM	1112	CZ	ARG A	152	23.188	29.662	41.577	1.00 16.78	A
ATOM	1113	NH1	ARG A	152	22.605	30.860	41.565	1.00 11.71	A
ATOM	1114	NH2	ARG A	152	23.885	29.265	40.518	1.00 11.02	Ā
ATOM	1115	С	ARG A	152	27.274	27.007	45.557	1.00 7.79	A
ATOM	1116	0	ARG A		26.671	26.313	46.389	1.00 5.08	A
ATOM	1117	N	PHE A	153	28.436	26.639	45.017	1.00 6.70	A
ATOM	1118	CA	PHE A		29.101	25.395	45.413	1.00 9.70	Ä
ATOM	1119	CB	PHE A		30.280	25.059	44.478	1.00 7.27	Ä
ATOM	1120	CG	PHE A		30.200	23.747	44.812	1.00 6.93	
ATOM	1121	CD1	PHE A		30.451	22.532	44.389		A
ATOM	1122	CD2	PHE A		32.134				A
ATOM	1123	CEI	PHE A			23.738	45.592	1.00 9.61	A
ATOM	1123				31.069	21.315	44.747	1.00 11.43	A
		CE2	PHE A		32.764	22.534	45.959	1.00 13.90	A
ATOM	1125	cz	PHE A		32.229	21.323	45.537	1.00 11.19	Ā
ATOM	1126	C	PHE A		29.640	25.503	46.842	1.00 8.50	A
ATOM	1127	O	PHE A		29.455	24.586	47.638	1.00 8.41	A
ATOM	1128	N	LEU A		30.320	26.599	47.167	1.00 6.84	A
MOTA	1129	CA	LEU A		30.877	26.752	48.521	1.00 6.20	A
ATOM	1130	CB	LEU A		31.672	28.060	48.657	1.00 6.23	A
ATOM	1131	CG	LEU A		32.876	28.250	47.720	1.00 6.30	A
MOTA	1132		LEU A		33.543	29.583	48.020	1.00 9.48	A
ATOM	1133		LEU A		33.893	27.117	47.886	1.00 6.15	A
ATOM	1134	С	LEU A		29.762	26.737	49.564	1.00 6.13	A
MOTA	1135	0	LEU A	154	29.912	26.170	50.641	1.00 9.16	A

ATOM	1136	N	ASN A	A 156	20 (52	00.004			
MOTA	1137	ĊA	ASN A		28.652		49.233		A
ATOM	1138	CB	ASN A		27.493	27.430	50.116		A
MOTA	1139	ĊĞ	ASN A		26.406	28.314	49.486		A
MOTA	1140	OD1			25.093	28.294	50.274	1.00 14.59	A
MOTA	1141	ND2		1 155	24.149	27.596	49.906	1.00 9.21	A
ATOM	1142	C	ASN A	1 155 1 155	25.034	29.062	51.361	1.00 8.23	A
ATOM	1143	ŏ	ASN A		26.929	26.042	50.363	1.00 8.76	A
MOTA	1144	N			26.465	25.712	51.465	1.00 8.00	A
ATOM	1145	CA	ALA A		26.965	25.203	49.336	1.00 8.80	A
ATOM	1146	CB	ALA A		26.418	23.867	49.493	1,00 7.63	A
ATOM	1147	C	ALA A		26.068	23.300	48.119	1.00 8.06	A
ATOM	1148	ŏ	ALA A		27.336	22.882	50.222	1.00 12.23	A
ATOM	1149	N	LYS A		26.854	22.037	50.994	1.00 9.62	A
ATOM	1150	CA	LYS A		28.646	23.029	50.015	1.00 9.93	A
ATOM	1151	CB	LYS A	157	29.623	22.064	50.537	1.00 10.69	Α
ATOM	1152	CG	LYS A	157	30.437	21.527	49.352	1.00 14.97	A
MOTA	1153	CD	LYS A		29.604	20.877	48.227	1.00 13.56	A
ATOM	1154	CE	LYS A		28.855	19.640	48.729	1.00 16.77	A
ATOM	1155	NZ	LYS A		28.357	18.784	47.575	1.00 22.67	A
ATOM	1156	C	LYS A		27.652	17.546	48.069	1.00 21.73	A
ATOM	1157	ŏ	LYS A	157	30.611	22.438	51.638	1.00 8.73	A
ATOM	1158	й	CYS A	150	31.215	21.552	52.245	1.00 11.63	A
ATOM	1159	CA	CYS A	150	30.821	23.725	51.876	1.00 8.12	A
ATOM	1160	Č.	CYS A	150	31.759 30.974	24.132	52.916	1.00 8.20	A
ATOM	1161	ŏ	CYS A			24.252	54.207	1.00 9.14	A
ATOM	1162	ČВ	CYS A		30.648	25.349	54.661	1.00 10.53	A
ATOM	1163	SG	CYS A		32.390 33.331	. 25.464	52.537	1.00 10.13	A
ATOM	1164	N	THR A		30.699	25.358	50.982	1.00 11.82	A _.
ATOM	1165	CA	THR A		29.856	23.108	54.822	1.00 8.92	A
MOTA	1166	CB	THR A		28.850	23.091	56.017	1.00 6.75	. <u>A</u>
ATOM	1167	0G1	THR A		29.551	21.933	55.903	1.00 10.13	A
ATOM	1168	CG2	THR A		28.146	20.690 21.989	55.987	1.00 12.88	A
ATOM	1169	Č	THR A		30.545	23.021	54.527	1.00 14.84	A
ATOM	1170	ŏ	THR A		29.878		57.361	1.00 8.62	Ä
ATOM	1171	N	THR A		31.875	22.956	58.398	1.00 7.39	A
ATOM	1172	ĈA	THR A		32.603	23.038	57.358	1.00 8.39	A
ATOM	1173	CB	THR A		33.194	22.980	58.612	1.00 9.53	A
ATOM	1174	OG1	THR A			21.558	58.889	1.00 8.99	A
ATOM	1175	CG2	THR A		34.011 32.083	21.140	57.788	1.00 12.55	A
ATOM	1176	C	THR A		33.727	20.559	59.114	1.00 11.60	Ā
ATOM	1177	ŏ	THR A		34.774	24.010	58.712	1.00 10.20	A
ATOM	1178	Ň	GLN A		33.523	23.739 25.189	59.314	1.00 8.76	A
ATOM	1179	CA	GLN A		34.525	26.260	58.121	1.00 8.66	A
ATOM	1180	CB	GLN A		34.564	27.121	58.254	1.00 9.46	Ā
MOTA	1181	CG	GLN A		34.956	26.309	56.989	1.00 9.58	Ā
ATOM	1182	CD	GLN A		36.305	25.608	55.742	1.00 7.83	A
MOTA	1183	OE1	GLN A		36.429	24.396	55.936 55.758	1.00 10.81 1.00 12.80	Ā
ATOM	1184	NE2	GLN A		37.306	26.374	56.313		A
MOTA	1185	C	GLN A		34.058	27.096	59.449	1.00 10.64	A
ATOM	1186	ŏ	GLN A		32.979	26.866	59.960	1.00 8.71 1.00 8.58	A
MOTA	1187	N		162	34.870	28.047	59.928	1.00 8.58 1.00 11.51	A
MOTA	1188	CD	PRO A	162	36.316	28.193	59.693	1.00 10.65	A
MOTA	1189	CA	PRO A	162	34.433	28.869	61.071	1.00 10.03	A
MOTA	1190	CB	PRO A		35.631	29.780	61.326	1.00 11.89	A
ATOM	1191	CG	PRO A		36.786	28.884	60.979	1.00 14.39	· A A
ATOM	1192	С	PRO A		33.171	29.660	60.727	1.00 10.67	Ä
ATOM	1193	0	PRO A		32.280	29.838	61.567	1.00 12.32	Ä
ATOM	1194	N	GLY A		33.112	30.158	59.492	1.00 12.32	A
ATOM	1195	CA	GLY A		31.943	30.903	59.040	1.00 11.83	A
ATOM	1196	C	GLY A	163	31.307	30.149	57.883	1.00 11.53	Ä
ATOM	1197	0	GLY A	163	31.687	28.989	57.628	1.00 9.27	Ā
ATOM	1198	N	THR A	164	30.359	30.781	57.178	1.00 7.79	Ä
ATOM	1199	CA	THR A	164	29.698	30.140	56.039	1.00 10.06	A
MOTA	1200	CB	THR A		28.213	29.775	56.347	1.00 10.00	A
MOTA	1201	OG1	THR A		27.565	30.914	56.934	1.00 12.97	A
MOTA	1202	CG2	THR A		28.119	28.585	57.328	1.00 7.94	A
MOTA	1203	C	THR A		29.696	31.081	54.837	1.00 10.41	A
MOTA	1204	0	THR A		29.786	32.301	55.001	1.00 7.96	A
MOTA	1205	N	PHE A		29.571	30.507	53.637	1.00 7.32	A
MOTA	1206	CA	PHE A	165	29.551	31.275	52.395	1.00 9.34	A
ATOM	1207	CB	PHE A	165	30.321	30.541	51.299	1.00 8.51	Â
MOTA	1208	CG	PHE A	165	31.799	30.451	51.539	1.00 7.69	Ä
MOTA	1209	CD1	PHE A	165	32.659	31.455	51.096	1.00 8.05	Ä
MOTA	1210		PHE A		32.338	29.338	52.181	1.00 10.52	Ä
MOTA	1211		PHE A		34.062	31.349	51.288	1.00 6.48	À
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ATOM MOTA	1212 1213	CE:			.720	29.214	52.385	1.00	6.44	A
ATOM ATOM	1214 1215	CZ C	PHE A 165 PHE A 165 PHE A 165	28	3.135	30.221	51.935 51.854	1.00	10.39	A A
ATOM ATOM	1216 1217	. N CA	ALA A 166 ALA A 166	27	7.428	30.485 32.712	51.648 51.601	1.00	8.80	A
MOTA MOTA	1218 1219	CB C	ALA A 166	25	.424	33.000 34.397	51.006 51.423	1.00	10.57	A A
ATOM ATOM	1220	0	ALA A 166 ALA A 166	27	.593	32.960 33.182	49.483 48.968	1.00	7.60	A A
MOTA	1221	N CA	VAL A 167 VAL A 167	25	.516 .572	32.668 32.658	48.766 47.303	1.00		A A
ATOM ATOM	1223 1224	CB CG1		24	.384	31.924 31.870	46.686 45.159	1.00		A A
ATOM ATOM	1225 1226	CG2	VAL A 167		.283	30.511 34.123	47.265 46.875	1.00	10.61	A A
MOTA MOTA	1227 1228	Ŋ	VAL A 167 THR A 168		.523	34.816 34.580	47.244 46.048	1.00	7.79	A A
ATOM ATOM	1229 1230	CA CB	THR A 168 THR A 168	26	.411	35.974 36.810	45.653 46.769	1.00	6.66	A A
MOTA MOTA	1231 1232	OG1	THR A 168	27	.129	38.188 36.311	46.370 47.040	1.00	12.35	A A
MOTA MOTA	1233 1234	C	THR A 168 THR A 168	27	.228	36.178 35.282	44.375	1.00	11.69	A A
MOTA MOTA	1235 1236	N CA	THR A 169 THR A 169	27	.106	37.352 37.641	43.770 42.580	1.00	9.36	A A
ATOM ATOM	1237 1238	CB OG1	THR A 169	27	.074	38.484 39.739	41.565	1.00	11.79	A
MOTA MOTA	1239 1240	CG2		25	.811	37.747 38.450	41.128 42.953	1.00	12.13	A A
ATOM ATOM	1241 1242	O N	THR A 169 VAL A 170	30	.000	38.712 38.848	42.099 44.224	1.00	8.64	A
ATOM ATOM	1243 1244	CA CB	VAL A 170 VAL A 170	30	.430	39.641 41.003	44.680	1.00	11.07	A
ATOM ATOM	1245 1246	CG1 CG2	VAL A 170	29	.433	41.863	45.248 44.106	1.00	8.12	A A
ATOM ATOM	1247	c o	VAL A 170 VAL A 170	31	.158	40.805 38.830 38.747	46.20B 45.741	1.00	10.94	A A
ATOM ATOM	1249 1250	N CA	PHE A 171 PHE A 171	32	.305	38.247	46.859 45.386	1.00		A
MOTA MOTA	1251 1252	CB CG	PHE A 171 PHE A 171	34	.003	37.367 36.775	46.312	1.00	9.52	A A
ATOM ATOM	1253 1254	CD1 CD2	PHE A 171	36	.940 .009 .457	35.686 35.978	46.519	1.00	9.84	A
ATOM ATOM	1255 1256	CE1 CE2	PHE A 171	36	.593	34.377 34.986	46.502 48.184	1.00	8.85	A A
MOTA MOTA	1257 1258	CZ	PHE A 171 PHE A 171	36	.096	33.377 33.686	47.311	1.00	12.76	A A
ATOM ATOM	1259 1260	Ŏ N	PHE A 171 ALA A 172	33	.292	37.977 37.294 39.257	47.661 48.679	1.00	7.64	A
ATOM ATOM	1261 1262	CA CB	ALA A 172 ALA A 172	34	.088 .655	39.865	47.677 48.946	1.00	6.57 9.02	A A
ATOM ATOM	1263 1264	C	ALA A 172 ALA A 172	32	. 948	41.279 39.885	48.721 49.957	1.00	9.26	A A
ATOM ATOM	1265 1266	N CA	ASN A 173 ASN A 173	31	.188	40.071 39.677	51.155 49.493	1.00	10.96 8.23	A A
ATOM ATOM	1267 1268	CB CG	ASN A 173 ASN A 173	29	.563 .361 .628	39.651 40.396	50.409 49.822	1.00	10.55	A
ATOM ATOM	1269 1270	OD1	ASN A 173	30.	. 28 9 . 09 8	41.862 42.512	49.606 50.412	1.00	13.88	A
ATOM ATOM	1271 1272	CO	ASN A 173 ASN A 173 ASN A 173	30.	. 06 2 . 07 7	42.398 38.245 38.109	48.515 50.759	1.00	16.29 13.21	A
MOTA MOTA	1273 1274	N CA	SER A 174 SER A 174	30.	. 71 6 . 25 0	37.212	51.498 50.238	1.00	7.67	A
ATOM ATOM	1275 1276	CB OG	SER A 174 SER A 174	30.	869	35.859 34.905	50.468 49.429	1.00	9.24 9.01	A A
ATOM ATOM	1277 1278	300	SER A 174 SER A 174	30.	.35 <i>9</i> .440 .480	33.580 35.250	49.598 51.863	1.00	8.15 7.73	A A
MOTA MOTA	1279 1280	N CA	TYR A 175 TYR A 175	31.	684	34.822 35.160	52.506 52.303	1.00	8.54 6.67	A A
ATOM ATOM	1281 1282	CB CG	TYR A 175 TYR A 175	33.	.978 .493 .928	34.535 34.371	53.599 53.735	1.00	6.35 7.83	A A
ATOM ATOM	1283 1284	CD1 CE1	TYR A 175 TYR A 175	34.	845	33.429 33.842	54.847 55.825	1.00	6.19 9.13	A A
ATOM ATOM	1285	CD2	TYR A 175	33.	315 481	32.938 32.102	56.811 54.879	1.00	7.78 6.63	A A
ATOM	1286 1287	CE2	TYR A 175 TYR A 175		93 <i>9</i> 85 <i>9</i>	31.206 31.633	55.856 56.812	1.00	9.07 11.83	A A

ATOM 1352 N VAL A 186 43.836 39.300 46.507 1.00 9.90 A ATOM 1353 CA VAL A 186 43.880 40.276 45.419 1.00 11.92 A ATOM 1355 CG1 VAL A 186 45.093 39.969 44.484 1.00 14.98 A ATOM 1355 CG1 VAL A 186 45.026 40.816 43.229 1.00 13.29 A ATOM 1356 CG2 VAL A 186 46.398 40.226 45.244 1.00 19.64 A ATOM 1357 C VAL A 186 42.608 40.254 44.571 1.00 11.79 A ATOM 1358 O VAL A 186 42.152 39.182 44.149 1.00 11.34 A ATOM 1359 N ALA A 187 42.035 41.430 44.331 1.00 11.06 A ATOM 1360 CA ALA A 187 40.829 41.543 43.508 1.00 10.57 A ATOM 1361 CB ALA A 187 39.897 42.606 44.096 1.00 12.53 A ATOM 1362 C ALA A 187 41.211 41.923 42.079 1.00 13.16									
ATOM 1289 C TYR A 1755 31.424 35.365 54.761 1.00 12.71 A ATOM 1291 O TYR A 1755 31.424 35.365 54.761 1.00 12.71 A ATOM 1292 O TYR A 1755 31.649 36.556 54.806 1.00 9.13 A ATOM 1292 CA SER A 1766 30.0695 34.727 55.683 1.00 9.13 A ATOM 1292 CA SER A 1766 30.0695 34.727 55.683 1.00 9.13 A ATOM 1295 C SER A 1766 30.073 31.433 55.7372 1.00 11.72 A ATOM 1295 C SER A 1766 30.073 34.433 55.7372 1.00 11.72 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1295 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1296 C SER A 1766 31.092 36.247 57.655 1.00 12.94 A ATOM 1296 C SER A 1767 31.303 36.559 58.561 1.00 12.94 A ATOM 1298 C SER A 1767 31.303 36.559 58.561 1.00 12.55 A ATOM 1300 C SEL EU A 1777 31.235 35.649 58.349 1.00 14.555 A ATOM 1301 C SEL EU A 1777 32.856 35.452 1.00 11.555 A ATOM 1302 C SEL EU A 1777 32.856 35.452 1.00 11.68 A ATOM 1304 C SEU A 1777 32.856 35.452 1.00 11.68 A ATOM 1305 C SEU A 1777 32.856 35.452 1.00 11.56 A ATOM 1306 C SEU A 1777 32.856 35.452 1.00 11.56 A ATOM 1307 C SEU A 1777 34.139 37.552 57.652 1.00 11.68 A ATOM 1308 C SEU A 1777 34.139 37.552 57.652 1.00 11.68 A ATOM 1307 C SEU A 1779 35.126 38.104 58.163 1.00 12.74 A ATOM 1308 C SEU A 1779 35.126 38.104 58.163 1.00 12.74 A ATOM 1307 C SEU A 1779 35.126 38.104 58.163 1.00 12.18 A ATOM 1307 C SEU A 1779 36.492 38.974 57.692 1.00 11.68 A ATOM 1308 C SEU A 1779 37.787 38.610 55.621 1.00 11.63 A ATOM 1309 N LEU A 1779 37.787 38.610 55.621 1.00 11.63 A ATOM 1309 N LEU A 1779 37.787 38.610 55.621 1.00 11.63 A ATOM 1309 N LEU A 1779 37.787 38.610 55.621 1.00 11.63 A ATOM 1309 C SER A 1800 39.906 38.399 55.208 1.00 11.63 A ATOM 1312 C SEU A 1779 37.787 39.90 37.799 40.017 49.994 1.00 12.85 A AT	ATOM	1288	ОН	TYR A 17	5 35 34 9	20 721	E7 746	1 00 0 05	
ATOM 1290 O TYR A 175 31.649 36.556 54.866 1.00 7.7.92 A ATOM 1292 N SER A 176 30.695 34.727 55.683 1.00 9.13 A ATOM 1292 C SER A 176 30.695 34.727 55.683 1.00 9.13 A ATOM 1293 C SER A 176 30.104 35.431 56.828 1.00 9.94 A ATOM 1294 C SER A 176 30.305 34.727 55.683 1.00 9.14 A ATOM 1295 C SER A 176 32.372 34.433 57.277 1.00 11.72 A ATOM 1295 C SER A 176 32.372 34.433 57.277 1.00 11.72 A ATOM 1295 C SER A 176 30.737 34.433 57.737 1.00 11.72 A ATOM 1295 C SER A 176 30.737 37.302 55.643 1.00 9.90 A ATOM 1295 C SER A 176 30.737 37.302 55.643 1.00 12.90 A ATOM 1297 N LEU A 177 32.332 35.787 57.788 1.00 10.90 A ATOM 1297 N LEU A 177 32.332 35.787 57.788 1.00 10.90 A ATOM 1297 N LEU A 177 32.332 35.787 57.788 1.00 10.90 A ATOM 1295 C LEU A 177 34.231 35.613 55.349 1.00 14.55 A ATOM 1290 C LEU A 177 34.231 35.613 55.349 1.00 11.72 A ATOM 1300 C LEU A 177 34.139 37.522 50.00 ATOM 1300 C LEU A 177 34.139 37.522 50.00 ATOM 1300 C LEU A 177 34.139 37.522 50.00 ATOM 1300 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1303 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1303 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1303 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1303 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1303 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1305 N GLU A 178 33.1546 38.645 58.645 1.00 12.71 A ATOM 1303 C LEU A 177 34.139 37.522 57.652 1.00 13.68 A ATOM 1305 N GLU A 178 33.645 36.693 37.652 57.652 1.00 13.68 A ATOM 1305 N GLU A 178 33.645 38.645 58.645 1.00 9.88 A ATOM 1305 N GLU A 178 33.645 38.645 58.645 1.00 9.88 A ATOM 1305 N GLU A 179 34.649 38.879 37.552 57.652 1.00 13.68 A ATOM 1308 C LEU A 179 36.693 38.693 39.404 58.163 1.00 12.71 A ATOM 1308 C LEU A 179 36.693 38.693 39.404 58.163 1.00 12.71 A ATOM 1308 C LEU A 179 36.693 38.693 39.503								_	
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ATOM 1356 CG2 VAL A 186 46.398 40.226 45.244 1.00 19.64 A ATOM 1357 C VAL A 186 42.608 40.254 44.571 1.00 11.79 A ATOM 1358 O VAL A 186 42.152 39.182 44.149 1.00 11.34 A ATOM 1359 N ALA A 187 42.035 41.430 44.331 1.00 11.06 A ATOM 1360 CA ALA A 187 40.829 41.543 43.508 1.00 10.57 A ATOM 1361 CB ALA A 187 39.897 42.606 44.096 1.00 12.53 A ATOM 1362 C ALA A 187 41.211 41.923 42.079 1.00 13.16	MOTA								
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	MOTA								
	MOTA								

ATOM	1364	N	ALA A 1	99	40.543	41 330	43 005		_
ATOM	1365	CA	ALA A 1		40.832	41.328 41.672	41.085	1.00 8.38	A
ATOM	1366	CB	ALA A 1		41.725		39.672	1.00 8.09	A
ATOM	1367	Č	ALA A 1			40.609	39.018	1.00 10.94	A
ATOM	1368	ŏ	ALA A 1		39.515	41.759	38.913	1.00 9.75	A
ATOM	1369	Ň	ILE A 1		38.510	41.196	39.349	1.00 10.74	A
ATOM	1370	CA	ILE A 1		39.543	42.434	37.766	1.00 10.19	Ä
ATOM	1371	CB			38.355	42.646	36.936	1.00 9.71	A
ATOM	1372	CG2		89 80	38.300	44.126	36.487	1.00 14.84	A
ATOM	1373	CG1			37.056	44.394	35.606	1.00 12.56	A
ATOM	1374	CD1			38.247	45.007	37.720	1.00 13.85	A
ATOM	1375	C	ILE A 1		36.964 38.307	44.848	38.520	1.00 20.17	A
MOTA	1376	ŏ	ILE A 1			41.760	35.705	1.00 11.18	A
ATOM	1377	N	GLY A 1		39.260 37.185	41.715	34.930	1.00 12.80	A
ATOM	1378	CA	GLY A 1			41.062	35.518	1.00 12.93	A
ATOM	1379	č	GLY A 1		37.039	40.181	34.368	1.00 9.66	A.
ATOM	1380	ŏ	GLY A 1		37.836 38.763	38.881	34.432	1.00 11.20	A
ATOM	1381	Ŋ	SER A 1		37.494	38.745	35.238	1.00 12.00	A
ATOM	1382	CA	SER A 1		38.216	37.919	33.570	1.00 12.31	A
MOTA	1383	CB	SER A 1		37.530	36.644	33.539	1.00 11.69	A
ATOM	1384	OG	SER A 1		36.224	35.671 35.299	32.568	1.00 8.59	A
ATOM	1385	Ċ	SER A 1		39.678	36.896	33.026 33.104	1.00 10.08	A
ATOM	1386	ō	SER A 1		40.612	36.295	33.638	1.00 14.30 1.00 11.39	A
ATOM	1387	N	VAL A 1		39.880	37.809	32.156	1.00 11.39	A
ATOM	1388	CA	VAL A 1		41.235	38.101	31.704	1.00 11.78	A
ATOM	1389	CB	VAL A 1		41.273	39.029	30.449	1.00 14.84	A A
ATOM	1390		VAL A 1	92	40.838	38.252	29.213	1.00 13.34	A
ATOM	1391	CG2			40.396	40.246	30.678	1.00 29.05	A
MOTA	1392	C	VAL A 1		42.056	38.767	32.804	1.00 11.65	Â
ATOM	1393	0	VAL A 1		43.247	38.485	32.940	1.00 14.10	Ä
ATOM	1394	N	GLY A 1	93	41.431	39.670	33.559	1.00 12.08	Ä
ATOM	1395	CA	GLY A 1	93	42.149	40.344	34.626	1.00 12.16	A
ATOM	1396	С	GLY A 1		42.575	39.354	35.700	1.00 14.30	Ä
ATOM	1397	0	GLY A 1	93	43.652	39.486	36.291	1.00 9.20	Ä
ATOM	1398	N	VAL A 1		41.725	38.369	35.976	1.00 9.32	Ä
ATOM	1399	CA	VAL A 1		42.069	37.370	36.992	1.00 9.16	A
ATOM	1400	CB	VAL A 1	94	40.845	36.459	37.341	1.00 7.74	A
ATOM	1401	CG1	VAL A 1	94	41.309	35.168	38.071	1.00 8.55	Ä
ATOM	1402	CG2	VAL A 1	94	39.873	37.247	38.259	1.00 11.33	Ä
ATOM	1403	С	VAL A 1	94	43.256	36.524	36.530	1.00 10.65	A
ATOM	1404	0	VAL A 1	94	44.158	36.255	37.318	1.00 10.00	A
MOTA	1405	N	MET A 1	95	43.261	36.090	35.265	1.00 9.82	A
ATOM	1406	CA	MET A 1	95	44.391	35.306	34.775	1.00 11.27	A
MOTA	1407	CB	MET A 1		44.125	34.727	33.381	1.00 13.33	A
ATOM	1408	CG	MET A 1		43.342	33.449	33.381	1.00 16.98	Α
MOTA	1409	SD	MET A 1		43.794	32.237	34.698	1.00 19.79	A
ATOM	1410	CE	MET A 1		45.205	31.419	34.043	1.00 16.46	Α
ATOM	1411	Č	MET A 1		45.672	36.118	34.719	1.00 12.67	A
ATOM	1412	0	MET A 1		46.757	35.579	34.948	1.00 15.56	A
ATOM	1413	N	ALA A 1		45.566	37.401	34.385	1.00 11.82	A
ATOM	1414	CA	ALA A 19		46.750	38.239	34.346	1.00 15.74	A
ATOM	1415	CB	ALA A 19		46.404	39.633	33.833	1.00 14.20	A
ATOM	1416	C	ALA A 19		47.331	38.323	35.768	1.00 16.81	A
ATOM	1417	O	ALA A 19		48.544	38.245	35.945	1.00 15.03	A
ATOM ATOM	1418	N	ALA A 19			38.468	36.778	1.00 13.86	A
	1419	CA	ALA A 19		46.939	38.538	38.151	1.00 13.25	A
ATOM ATOM	1420	CB C	ALA A 19		45.790	38.865	39.108	1.00 13.70	Ā
	1421 1422	_	ALA A 19	7 /	47.547	37.203	38.542	1.00 13.49	Ā
ATOM		O	ALA A 19		48.618	37.159	39.147	1.00 13.32	Ā
ATOM ATOM	1423 1424	N CA	ASP A 19		46.853	36.119	38.202	1.00 12.41	Ā
ATOM	1425	CB	ASP A 19	70	47.326	34.777	38.547	1.00 16.61	A
ATOM	1425		ASP A 13	20	46.311	33.719	38.074	1.00 18.96	A
ATOM	1426	CG	ASP A 19		46.605	32.327	38.629	1.00 29.19	A
					46.440	32.107	39.857	1.00 32.24	Ā
ATOM ATOM	1428 1429		ASP A 19		47.004	31.449	37.834	1.00 34.04	A
ATOM	1429	C	ASP A 19		48.699	34.509	37.928	1.00 17.95	A
	1431	O N	ASP A 19		49.570	33.942	38.585	1.00 18.27	A
ATOM		N Ca	ASN A 19		48.900	34.941	36.684	1.00 16.24	À
ATOM	1432	CA	ASN A 19		50.173	34.733	35.980	1.00 17.75	A
ATOM	1433 1434	CB CG	ASN A 19		49.941	34.565	34.478	1.00 19.50	A
ATOM ATOM	1434		ASN A 19		49.270	33.263	34.122	1.00 21.16	A
ATOM	1435	ND2	ASN A 19		49.454	32.254	34.786	1.00 29.31	A
ATOM	1437	C	ASN A 19		48.504 51.227	33.275 35.832	33.041	1.00 24.39	A
ATOM	1438	ŏ	ASN A 19		52.272	35.762	36.144	1.00 20.64	A
ATOM	1439	Ŋ	ASP A 20		50.973	36.838	35.507 36.970	1.00 27.47	A
111011	× 2 J J	74	1. 20		30.373	20.030	30.7/0	1.00 19.22	A

ATOM	1440 1441	CA	ASP A 200		. 925	37.937	37.148		20.54	Ā
ATOM ATOM ATOM	1442 1443	CB CG OD1	ASP A 200 ASP A 200 ASP A 200	52	.350 .166 .356	38.985 40.271 40.256	38.092 38.105 37.713	1.00		A A A
MOTA MOTA	1444	OD2 C		51	.612	41.296 37.431	38.526 37.716	1.00	26.57	A A
ATOM MOTA	1446 1447	Ŏ N	ASP A 200 VAL A 201	53	.315	36.967 37.511	38.855 36.922	1.00	19.25	A A
ATOM ATOM	1448 1449	CA CB	VAL A 201 VAL A 201	55	.611	37.033 36.597	37.390 36.216	1.00		A A
ATOM ATOM	1450 1451	CG1 CG2	VAL A 201	55	.910	35.377 37.754	35.519 35.246	1.00		A A
ATOM ATOM	1452 1453	C	VAL A 201 VAL A 201	56	.370	38.046 37.744	38.222 38.715	1.00		A A
ATOM MOTA	1454 1455	N CA	THR A 202 THR A 202	55	.817	39.241 40.251	38.402 39.190	1.00		A A
ATOM ATOM	1456 1457	CB OG1	THR A 202	56	.216	41.664 41.999	38.696 38.979	1.00	22.33	A A
ATOM ATOM	1458 1459	CG2 C	THR A 202 THR A 202	56	.489	41.759 40.184	37.210 40.677	1.00		A A
ATOM ATOM	1460 1461	O N	THR A 202 THR A 203	56	.543 .440	41.073 39.147	41.444 41.076	1.00	25.68 19.97	A A
MOTA MOTA	1462 1463	CA CB	THR A 203 THR A 203	55	.116	38.957 39.167	42.484	1.00	20.69	A
ATOM ATOM	1464 1465	OG1 CG2			.825 .202	38.196 40.581	42.047 42.363	1.00	25.13	A A
ATOM ATOM	1466 1467	C O	THR A 203 THR A 203	55	.523 .771	37.521 36.703	42.834 41.947	1.00		A A
ATOM ATOM	1468 1469	N CA	ALA A 204 ALA A 204	56	.624 .011	37.217 35.867	44.116 44.528	1.00 1.00	16.26	, A A
ATOM ATOM	1470	CB C	ALA A 204 ALA A 204	54	.175 .978	35.825 34.832	46.065 44.092	1.00		A A
ATOM ATOM	1472	O N	ALA A 204 GLN A 205	55	.806	35.157 33.582	43.906 43.921	1.00		A A
MOTA MOTA MOTA	1474 1475 1476	CA CB CG	GLN A 205 GLN A 205 GLN A 205	55	.483	32.501 31.191	43.560 43.316	1.00		A A
ATOM ATOM	1477 1478	CD OE1	GLN A 205	56	.103 .469 .446	31.148 29.716 28.801	42.097 41.717 42.565	1.00	22.41 29.28 20.67	A A
ATOM ATOM	1479 1480	NE2 C		56	.813	29.510 32.262	40.442 44.728		25.77 14.53	A A A
ATOM ATOM	1481 1482	о И	GLN A 205 GLY A 206	53	.783	32.717 31.540	45.846 44.478	1.00	14.81	Ä
ATOM ATOM	1483 1484	CA C	GLY A 206 GLY A 206	51	.509 .042	31.236 31.518	45.554 45.284	1.00	11.46	A A
MOTA MOTA	1485 1486	N N	GLY A 206 ARG A 207	49	.162 .764	31.067 32.236	46.046 44.199	1.00	9.87 7.71	A A
ATOM ATOM	1487 1488	CA CB	ARG A 207 ARG A 207	48	. 38 3 . 36 4	32.606 33.763	43.878 42.863	1.00	7.50 9.66	A A
ATOM ATOM	1489 1490	CG CD	ARG A 207 ARG A 207	48	.719 .774	35.114 36.286	43.493 42.497	1.00 1.00	7.35 6.76	A A
MOTA MOTA	1491 1492	NE CZ	ARG A 207 ARG A 207	49	.079 .156	37.532 38.738	43.221 42.654	1.00	10.86 13.78	A A
MOTA MOTA	1493 1494	NH1 NH2	ARG A 207	49	.957 .415	38.881	41.350 43.398	1.00	9.77 15.04	A A
ATOM ATOM ATOM	1495 1496 1497	С 0 N	ARG A 207 ARG A 207 ILE A 208	47	.500 .959 .214	31.475 30.549 31.572	43.389	1.00 1.00 1.00	11.20	A A
ATOM ATOM	1498 1499	CA CB	ILE A 208 ILE A 208	45	.245	30.557 29.491	43.721 43.331 44.476	1.00	8.65 8.62 11.42	A A A
ATOM ATOM	1500 1501	CG2 CG1	ILE A 208	44	.533	30.157	45.766 43.984	1.00	8.84 12.09	A A
ATOM ATOM	1502 1503	CD1 C		44	.207	27.094 31.286	44.823 43.056	1.00	11.77	A A
ATOM ATOM	1504 1505	O N	ILE A 208 THR A 209	43	.664 .098	32.335 30.776	43.649 42.145		12.81 7.78	A
ATOM ATOM	1506 1507	CA CB	THR A 209 THR A 209		.825 .055	31.470 32.610	41.864 40.849	1.00	9.01 11.48	A
ATOM ATOM	1508 1509	OG1 CG2		42	.906 .310	33.455 32.030	40.789 39.460	1.00	11.18 12.27	A A
ATOM ATOM	1510 1511	CO	THR A 209 THR A 209	40	.751 .978	30.534 29.326	41.319	1.00	10.48	A A
ATOM	1512 1513	N CA	TYR A 210 TYR A 210	38	.577 .476	31.087 30.303	40.997	1.00	8.58 8.34	A A
ATOM ATOM	1514 1515	CB CG	TYR A 210 TYR A 210		. 24 4 . 68 5	30.304 31.664	41.350 41.695	1.00	4.35 7.98	A A

ATOM ATOM ATOM ATOM ATOM ATOM	1516 1517 1518 1519 1520 1521	CD1 CE1 CD2 CE2 CZ OH	TYR A TYR A TYR A	210 210 210 210	35.656 35.153 37.188 36.699 35.687 35.242	32.240 33.509 32.386 33.643 34.203 35.475	40.927 41.235 42.778 43.086 42.313 42.598	1.00 6.11 1.00 7.73 1.00 6.57 1.00 5.93 1.00 8.47 1.00 8.24	A A A A
ATOM ATOM ATOM	1522 1523 1524 1525	C O N CA	TYR A TYR A ILE A ILE A	210 211	38.169 38.184 37.934 37.720	30.983 32.222 30.201 30.832	39.087 39.010 38.032 36.735	1.00 5.52 1.00 9.37 1.00 6.28	A A A
ATOM ATOM ATOM	1526 1527 1528	CB CG2 CG1	ILE A	211 211	39.085 39.990 38.902	31.384 30.231 32.361	36.235 35.830 35.075	1.00 7.52 1.00 11.97 1.00 10.21 1.00 14.62	A A A
ATOM ATOM	1529 1530 1531	CD1 C O	ILE A ILE A ILE A	211 211 211	40.159 37.132 37.080	33.203 29.936 28.703	34.806 35.648 35.778	1.00 15.71 1.00 8.22 1.00 8.13	A A A
ATOM ATOM ATOM ATOM	1532 1533 1534 1535	N CA CB OG	SER A SER A	212	36.634 36.140 35.984	30.590 29.913 30.934	34.602 33.394 32.256	1.00 9.06 1.00 9.98 1.00 8.45	A A A
ATOM ATOM ATOM	1536 1537 1538	00 N	SER A SER A PRO A	212 212	35.637 37.181 38.361 36.761	30.283 28.904 29.234 27.668	31.037 32.914 32.812 32.585	1.00 9.53 1.00 10.00 1.00 7.50 1.00 8.50	A A A
ATOM ATOM ATOM	1539 1540 1541	CD CA CB	PRO A PRO A	213 213 213	35.436 37.781 37.035	27.030 26.728 25.392	32.686 32.117 32.059	1.00 8.50 1.00 4.78 1.00 8.39 1.00 10.29	A A A
ATOM ATOM ATOM ATOM	1542 1543 1544 1545	CG C	PRO A PRO A	213 213	35.578 38.360 39.433	25.849 27.149 26.698	31.743 30.777 30.390	1.00 9.33 1.00 10.79 1.00 10.83	A A A
ATOM ATOM ATOM	1546 1547 1548	N CA CB CG	ASP A ASP A ASP A	214 214	37.668 38.164 37.033 37.248	28.038 28.514 29.175 29.146	30.074 28.775 27.997 26.497	1.00 5.80 1.00 8.50 1.00 7.35 1.00 11.12	A A A
ATOM ATOM ATOM	1549 1550 1551	OD1 OD2 C	ASP A	214 214	36.479 38.159 39.314	29.849 28.428 29.526	25.801 26.007 28.935	1.00 11.42 1.00 10.72 1.00 12.08	A A A
ATOM ATOM ATOM	1552 1553 1554 1555	O N CA CB	ASP A PHE A PHE A	215 215	39.933 39.572 40.662 40.121	29.931 29.958 30.901 32.106	27.943 30.170 30.459 31.233	1.00 13.08 1.00 9.47 1.00 9.63 1.00 12.63	A A A
ATOM ATOM ATOM	1556 1557 1558	CD2	PHE A PHE A PHE A	215 215 215	39.375 39.957 38.074	33.081 34.301 32.812	30.402 30.067 29.986	1.00 9.86 1.00 11.72 1.00 11.34	A A A
ATOM ATOM ATOM ATOM	1559 1560 1561 1562	CE1 CE2 CZ C	PHE A PHE A PHE A	215 215	39.250 37.357 37.949 41.748	35.250 33.759 34.976 30.286	29.332 29.245 28.921 31.356	1.00 11.89 1.00 6.37 1.00 13.90 1.00 13.88	A A A
ATOM ATOM ATOM	1563 1564 1565	O N CA	PHE A ALA A ALA A	215 216 216	42.837 41.463 42.404	30.865 29.131 28.535	31.480 31.976 32.936	1.00 12.28 1.00 9.02 1.00 9.41	A A A
ATOM ATOM ATOM ATOM	1566 1567 1568 1569	C O C B	ALA A : ALA A : ALA A :	216 216	41.705 43.727 44.679 43.790	27.432 28.007 27.844 27.719	33.753 32.406 33.178 31.106	1.00 9.18 1.00 13.18 1.00 16.82 1.00 12.39	A A A A
ATOM ATOM ATOM	1570 1571 1572	CA CB C	ALA A : ALA A :	217 217 217	45.031 45.094 45.136	27.224 25.693 27.660	30.522 30.625 29.063	1.00 14.59 1.00 15.34 1.00 16.52	A A A
ATOM ATOM ATOM ATOM	1573 1574 1575 1576	O N CD CA	PRO A : PRO A : PRO A :	218 218	44.128 46.358 47.657 46.533	27.958 27.690 27.532 28.101	28.418 28.517 29.194 27.111	1.00 14.71 1.00 18.85 1.00 19.53 1.00 17.17	A A A
ATOM ATOM ATOM ATOM	1577 1578 1579 1580	CB CG C	PRO A PRO A PRO A	218 218	48.053 48.553 45.889	28.171 28.433 27.162	26.952 28.357 26.076	1.00 22.03 1.00 24.10 1.00 17.95	A A A
ATOM ATOM ATOM	1581 1582 1583	O N CA CB	SER A SER A SER A	219 219	45.490 45.804 45.212 46.308	27.606 25.872 24.883 24.053	24.986 26.395 25.490 24.816	1.00 20.60 1.00 12.39 1.00 11.61 1.00 17.69	A A A
ATOM ATOM ATOM ATOM	1584 1585 1586 1587	OG C O N	SER A	219 219	46.870 44.341 44.454 43.479	23.140 23.942 23.896 23.180	25.749 26.324 27.559	1.00 17.25 1.00 14.52 1.00 15.86	A A A
ATOM ATOM ATOM ATOM	1588 1589 1590 1591	CA CB CG	LEU A LEU A LEU A	220 220 220	42.614 41.705 40.632 39.908	22.250 21.491 22.337 21.517	25.664 26.389 25.401 24.707 23.646	1.00 13.85 1.00 13.63 1.00 15.59 1.00 16.07 1.00 15.58	A A A A

ATOM	1592	CD2	LEU A	320	20 625	22 055	25 752	1 00 16 22	7
ATOM	1593	Č	LEU		39.635 43.401	22.855 21.251	25.752 27.245	1.00 16.33 1.00 15.71	A A
ATOM	1594	ŏ	LEU A		43.034	20.986	28.395	1.00 15.65	A
ATOM	1595	Ň	ALA A		44.481	20.693	26.698	1.00 15.60	A
ATOM	1596	ĊA	ALA A		45.283	19.714	27.452	1.00 18.03	A
MOTA	1597	CB	ALA A		46.452	19.175	26.604	1.00 17.58	A
ATOM	1598	Ċ	ALA A		45.834	20.298	28.738	1.00 17.30	À
ATOM	1599	ŏ	ALA A		46.085	19.573	29.687	1.00 15.45	Ā
ATOM	1600	N	GLY A		46.038	21.612	28.754	1.00 15.25	A
ATOM	1601	CA	GLY A		46.561	22.267	29.947	1.00 11.71	Ä
ATOM	1602	C	GLY A		45.641	22.101	31.144	1.00 10.72	Ä
ATOM	1603	0	GLY A		46.105	22.139	32.280	1.00 14.13	A
ATOM	1604	N	LEU A		44.340	21.938	30.914	1.00 11.19	A
ATOM	1605	CA	LEU A	223	43.406	21.751	32.033	1.00 8.14	А
ATOM	1606	CB	LEU A		41.946	21.728	31.525	1.00 9.90	A
ATOM	1607	CG	LEU A		41.481	23.046	30.874	1.00 9.91	A
ATOM	1608		LEU A		40.035	22.918	30.331	1.00 9.85	A
ATOM	1609	CD2	LEU A		41.570	24.153	31.926	1.00 9.05	A
ATOM	1610	C	LEU A		43.720	20.444	32.773	1.00 11.22	. A
ATOM ATOM	1611 1612	N O	LEU A		43.369	20.297	33.939	1.00 7.21	Ä
ATOM	1613	CA	ASN A		44.389 44.742	19.505	32.100	1.00 9.60	A
ATOM	1614	CB	ASN A		44.651	18.231 17.078	32.727 31.706	1.00 10.35 1.00 13.70	A A
ATOM	1615	CG	ASN A		43.214	16.768	31.301	1.00 15.75	A
ATOM	1616	OD1	ASN A		42.347	16.610	32.146	1.00 21.72	A
ATOM	1617		ASN A		42.968	16.666	30.012	1.00 14.86	Ä
ATOM	1618	C	ASN A		46.138	18.239	33.359	1.00 12.93	A
ATOM	1619	0	ASN A		46.580	17.226	33.898	1.00 14.86	A
MOTA	1620	N	ASP A	225	46.833	19.370	33.308	1.00 8.74	A
ATOM	1621	CA	ASP A		48.163	19.437	33.932	1.00 12.69	A
ATOM	1622	CB	ASP A		49.031	20.467	33.199	1.00 11.40	A
ATOM	1623	CG	ASP A		50.402	20.654	33.843	1.00 15.89	A
ATOM ATOM	1624	OD1 OD2			50.673	20.076	34.922	1.00 14.10	A
ATOM	1625 1626	C C	ASP A		51.211	21.401	33.261	1.00 16.19	A
MOTA	1627	ŏ	ASP A		47.960 47.776	19.844 21.016	35.398 35.691	1.00 13.53 1.00 10.79	A
ATOM	1628	Ň	ALA A		48.035	18.882	36.317	1.00 10.79 1.00 10.49	A A
ATOM	1629	CA	ALA A		47.792	19.178	37.720	1.00 10.49	À
ATOM	1630	CB	ALA A		47.424	17.889	38.478	1.00 13.20	Ä
ATOM	1631	C	ALA A		48.881	19.939	38.461	1.00 12.23	Ä
ATOM	1632	0	ALA A	226	48.773	20.144	39.678	1.00 13.15	A
ATOM	1633	N	THR A	227	49.935	20.347	37.762	1.00 10.64	A
MOTA	1634	CA	THR A		50.955	21.148	38.426	1.00 10.50	A
ATOM	1635	CB	THR A		52.405	20.854	37.917	1.00 15.63	A
ATOM	1636	OG1	THR A		52.541	21.287	36.561	1.00 13.88	Ā
ATOM ATOM	1637 1638	CG2 C	THR A		52.718	19.374	38.009	1.00 16.59	A
ATOM	1639	ŏ	THR A		50.620 51.320	22.628 23.509	38.154 38.626	1.00 9.17 1.00 10.52	A A
ATOM	1640	Ň	LYS A		49.530	22.876	37.414	1.00 10.32	Ä
ATOM	1641	CA	LYS A		49.079	24.226	37.069	1.00 12.05	Ä
ATOM	1642	CB	LYS A		49.378	24.511	35.594	1.00 15.38	A
MOTA	1643	CG	LYS A		50.877	24.607	35.272	1.00 22.71	A
ATOM	1644	CD	LYS A	228	51.125	24.652	33.758	1.00 20.66	Α
ATOM	1645	CE		228	52.613	24.720	33.447	1.00 26.84	A
ATOM	1646	NZ	LYS A		53.205	25.974	33.986	1.00 37.16	A
ATOM	1647	Č	LYS A		47.576	24.453	37.313	1.00 8.78	A
ATOM	1648	0	LYS A		47.153	25.574	37.634	1.00 9.99	A
ATOM	1649	N	VAL A		46.777	23.407	37.100	1.00 9.98	A
ATOM ATOM	1650 1651	CA CB	VAL A		45.327	23.465	37.282	1.00 6.71	A
ATOM	1652	CG1	VAL A		44.611 43.082	23.300 23.303	35.939	1.00 8.87	A
ATOM	1653	CG2	VAL A		45.019	24.468	36.150	1.00 10.77 1.00 10.90	A A
ATOM	1654	C	VAL A		44.913	22.339	34.988 38.245	1.00 10.50	A
MOTA	1655	ō	VAL A		45.107	21.154	37.967	1.00 8.04	Ä
MOTA	1656	Ň	ALA A		44.343	22.706	39.383	1.00 10.29	Ä
MOTA	1657	CA	ALA A		43.985	21.696	40.387	1.00 8.30	Ä
MOTA	1658	CB	ALA A		43.612	22.380	41.677	1.00 10.71	A
MOTA	1659	C	ALA A		42.900	20.691	40.064	1.00 12.18	A
MOTA	1660	0	ALA A		41.884	21.020	39.435	1.00 12.58	A
MOTA	1661	N	ARG A		43.120	19.452	40.501	1.00 8.23	Ā
ATOM	1662	CA	ARG A		42.080	18.436	40.382	1.00 8.98	A
MOTA	1663	CB	ARG A		42.656	17.021	40.495	1.00 11.67	A
MOTA MOTA	1664 1665	CG CD	ARG A		43.433 44.130	16.581 15.244	39.265	1.00 14.58	A
ATOM	1666	NE	ARG A		44.130	15.244	39.487 38.336	1.00 18.76 1.00 19.63	A A
ATOM	1667	CZ	ARG A		45.931	14.029	38.331	1.00 19.63	A

ATOM 1669 NH2 ARG A 231	ATOM	1668	NH1	ARG A	231	46.184	13.312	39.426	1.00 22.17	A
ATOM 1671 O ARG A 231 11.801 19.332 42.582 1.00 13.24 A ATOM 1672 N THR A 232 39.807 18.371 41.640 1.00 9.11 A ATOM 1673 CA THR A 232 39.80 18.607 42.822 1.00 11.84 A ATOM 1676 CGZ THR A 232 39.80 18.607 42.822 1.00 11.84 A ATOM 1676 CGZ THR A 232 39.807 19.807 14.602 1.00 11.64 A ATOM 1676 CGZ THR A 232 39.807 19.807 14.603 1.00 17.60 1.00 17.60 A ATOM 1676 CGZ THR A 232 39.807 17.351 31.001 17.60 1.00 17.60 A ATOM 1676 CGZ THR A 232 39.807 17.351 31.001 17.60 A ATOM 1677 C THR A 232 37.869 16.747 42.118 1.00 13.13 A ATOM 1679 N GLU A 233 37.869 16.747 42.118 1.00 13.13 A ATOM 1679 N GLU A 233 37.869 16.747 42.118 1.00 13.13 A ATOM 1679 N GLU A 233 37.869 16.747 42.118 1.00 13.13 A ATOM 1682 C GLU A 233 37.869 16.747 42.118 1.00 13.157 A ATOM 1682 C GLU A 233 37.869 16.747 42.118 1.00 13.157 A ATOM 1682 C GLU A 233 37.869 16.747 42.118 1.00 13.157 A ATOM 1682 C GLU A 233 39.460 14.831 45.706 1.00 14.67 A ATOM 1682 C GLU A 233 39.460 14.831 45.706 1.00 14.67 A ATOM 1682 C GLU A 233 4 39.460 14.831 45.706 1.00 14.67 A ATOM 1685 C GLU A 233 4 41.577 14.442 46.830 1.00 13.37 A ATOM 1685 C GLU A 233 4 41.577 14.442 46.830 1.00 13.37 A ATOM 1688 C GLU A 233 4 41.577 14.442 46.830 1.00 13.37 A ATOM 1689 NZ LYS A 234 41.574 11.577 14.442 46.830 1.00 13.47 A ATOM 1689 NZ LYS A 234 41.594 13.576 48.839 1.00 15.76 A ATOM 1689 C GLU A 233 39.860 13.576 48.839 1.00 15.76 A ATOM 1689 C GLU A 233 39.860 13.576 48.839 1.00 15.76 A ATOM 1689 C GLU A 233 39.860 13.576 48.839 1.00 12.77 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C GLU A 235 39.866 12.224 48.031 1.00 15.86 A ATOM 1690 C GLU A 235 39.866 12.224 48.031 1.00 12.77 A ATOM 1691 C LYS A 234 39.856 13.846 14.240 48.851 1.00 15.86 A ATOM 1691 C LYS A 234 39.856 13.846 14.240 48.851 1.00 12.77 A ATOM 1693 C GLU A 235 39.866 14.240 48.851 1.00 12.79 A ATOM 1693 C GLU A 238 39.866 14.240 48.851 1.00 12.79 A ATOM 1693 C GLU A 234 39.858 1.0			_						1.00 31.31	A
ATOM 1672 N THR A 232 39.997 18.371 41.640 1.00 9.11 A ATOM 1673 CA THR A 232 39.180 18.607 42.822 1.00 11.84 A ATOM 1673 CA THR A 232 39.180 18.607 42.822 1.00 11.84 A ATOM 1676 CG THR A 232 39.180 19.820 42.623 1.00 13.64 A ATOM 1676 CG THR A 232 37.869 19.820 42.623 1.00 13.64 A ATOM 1676 CG THR A 232 37.869 16.747 42.188 1.00 17.60 A ATOM 1677 C THR A 232 37.869 16.747 42.188 1.00 13.36 A ATOM 1678 O THR A 232 37.869 16.747 42.118 1.00 9.412 A ATOM 1679 N GLY A 233 38.357 17.551 43.071 1.00 9.55 A ATOM 1679 N GLY A 233 38.40 16.934 44.332 1.00 9.55 A ATOM 1680 CA GLY A 233 38.40 16.934 44.332 1.00 9.55 A ATOM 1681 N GLY A 233 38.40 16.934 44.332 1.00 9.55 A ATOM 1682 N GLY A 233 38.40 16.934 44.332 1.00 13.57 A ATOM 1682 N GLY A 233 38.40 16.934 44.335 1.00 13.57 A ATOM 1682 N GLY A 233 38.40 16.934 44.335 1.00 15.04 A ATOM 1682 N GLY A 233 38.40 18.87 14.616 45.366 1.00 14.09 A ATOM 1682 N GLY A 234 40.226 13.834 46.438 1.00 15.04 A ATOM 1685 CB LYS A 234 40.226 13.834 46.830 1.00 13.37 A ATOM 1686 CG LYS A 234 42.831 13.576 47.688 1.00 14.40 A ATOM 1686 CG LYS A 234 42.801 13.576 47.688 1.00 13.37 A ATOM 1685 CB LYS A 234 42.801 14.314 47.968 1.00 17.84 A ATOM 1689 N LYS A 234 43.807 18.314 47.666 18.81 N LYS A 234 A ATOM 1689 N LYS A 234 43.807 18.314 47.666 18.81 N LYS A 234 A ATOM 1689 N LYS A 234 43.807 18.314 47.666 19.81 N LYS A 234 A ATOM 1689 N LYS A 234 43.807 18.314 47.696 1.00 17.96 A ATOM 1689 N LYS A 234 43.807 18.314 47.696 1.00 17.96 A ATOM 1689 N LYS A 234 43.807 18.314 47.696 1.00 17.96 A ATOM 1689 N LYS A 234 43.807 18.314 47.696 1.00 17.96 A ATOM 1699 N LYS A 234 43.807 18.314 47.696 1.00 17.96 A ATOM 1699 N LYS A 234 38.885 11.694 49.223 1.00 17.517 A ATOM 1698 N LYS A 234 38.885 11.694 49.223 1.00 17.91 A ATOM 1698 N LYS A 234 38.885 11.694 49.223 1.00 17.91 A ATOM 1695 N LYS A 234 38.885 11.694 49.223 1.00 17.91 A ATOM 1695 N LYS A 234 38.895 11.694 49.223 1.00 17.95 A ATOM 1695 N LYS A 234 38.895 11.694 49.223 1.00 17.95 A ATOM 1695 N LYS A 234 38.895 18.895 18.895 18.995 18.00 17.9	_ :									
ATOM 1674 CB THR A 232 38.236 19.820 42.823 1.00 11.64 A ATOM 1675 CGI THR A 232 39.017 21.004 42.384 1.00 11.66 A ATOM 1676 CGZ THR A 232 37.382 20.025 43.883 1.00 11.43 A ATOM 1677 C THR A 232 37.382 20.025 43.883 1.00 11.43 A ATOM 1677 C THR A 232 38.357 17.351 43.071 1.00 9.12 A ATOM 1677 C THR A 232 38.357 17.351 43.071 1.00 9.12 A ATOM 1680 CD THR A 233 37.869 16.747 42.118 1.00 13.13 A ATOM 1680 CD CLY A 233 37.869 16.747 42.118 1.00 13.13 A ATOM 1680 CD CLY A 233 38.547 11.516 45.564 1.00 14.59 A ATOM 1680 CD CLY A 233 39.460 14.831 45.706 1.00 14.59 A ATOM 1681 CD CLY A 233 39.640 14.831 45.706 1.00 14.67 A ATOM 1682 CD CLY A 233 39.640 14.831 45.706 1.00 14.67 A ATOM 1683 N LYS A 234 40.226 13.834 46.438 1.00 15.04 A ATOM 1685 CD LYS A 234 41.577 14.442 46.830 1.00 13.37 A ATOM 1685 CD LYS A 234 41.577 14.442 46.830 1.00 13.37 A ATOM 1685 CD LYS A 234 41.577 14.442 46.830 1.00 13.37 A ATOM 1688 CC LYS A 234 41.594 13.567 47.688 1.00 14.00 A ATOM 1689 NZ LYS A 234 41.594 13.567 48.839 1.00 15.58 A ATOM 1689 NZ LYS A 234 41.594 13.567 48.839 1.00 15.58 A ATOM 1698 NZ LYS A 234 41.594 13.867 48.839 1.00 15.78 A ATOM 1690 C LYS A 234 49.765 13.414 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1690 C LYS A 234 39.450 13.411 47.697 1.00 17.96 A ATOM 1697 CA SER A 236 37.811 9.99 1.00 12.40 13.77 A ATOM 1697 CA SER						39.997	18.371	41.640	1.00 9.11	A
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ATOM 1688 CE LYS A 234				LYS A	234	42.483	13.576	47.688	1.00 14.40	
ATOM 1689 NZ LYS A 234										
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ATOM 1733 CB GLU A 243 42.444 10.473 42.132 1.00 23.30 A ATOM 1734 CG GLU A 243 43.643 9.624 42.499 1.00 31.37 A ATOM 1735 CD GLU A 243 44.658 9.584 41.368 1.00 37.64 A ATOM 1736 OE1 GLU A 243 44.234 9.507 40.195 1.00 38.59 A ATOM 1737 OE2 GLU A 243 45.876 9.628 41.644 1.00 41.94 A ATOM 1738 C GLU A 243 40.469 11.817 42.757 1.00 15.80 A ATOM 1739 O GLU A 243 39.417 11.406 42.285 1.00 17.65 A ATOM 1740 N GLY A 244 40.765 13.111 42.827 1.00 15.34 A ATOM 1741 CA GLY A 244 39.832 14.101 42.286 1.00 16.23 A ATOM 1742 C GLY A 244 39.994 14.161 40.770 1.00 16.48										
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ATOM 1737 OE2 GLU A 243 45.876 9.628 41.644 1.00 41.94 A ATOM 1738 C GLU A 243 40.469 11.817 42.757 1.00 15.80 A ATOM 1739 O GLU A 243 39.417 11.406 42.285 1.00 17.65 A ATOM 1740 N GLY A 244 40.765 13.111 42.827 1.00 15.34 A ATOM 1741 CA GLY A 244 39.832 14.101 42.286 1.00 16.23 A ATOM 1742 C GLY A 244 39.994 14.161 40.770 1.00 16.48 A										
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ATOM 1740 N GLY A 244 40.765 13.111 42.827 1.00 15.34 A ATOM 1741 CA GLY A 244 39.832 14.101 42.286 1.00 16.23 A ATOM 1742 C GLY A 244 39.994 14.161 40.770 1.00 16.48 A										
ATOM 1741 CA GLY A 244 39.832 14.101 42.286 1.00 16.23 A ATOM 1742 C GLY A 244 39.994 14.161 40.770 1.00 16.48 A										
									1.00 16.23	A

MOTA	1744	N	LYS A 245	39.148	14.939	40.096	1.00 14.99	A
ATOM	1745	CA	LYS A 245	39.186	15.079	38.632	1.00 14.88	A
MOTA	1746	CB	LYS A 245	37.792	14.795	38.060	1.00 13.06	A
MOTA	1747	CG	LYS A 245	37.294	13.363	38.289	1.00 22.95	Ä
ATOM	1748	CD	LYS A 245	38.174	12.353	37.540	1.00 27.44	Â
ATOM	1749	CE	LYS A 245	37.596	10.939	37.643		
ATOM	1750	NZ	LYS A 245				1.00 27.64	A
ATOM	1751	C	LYS A 245	37.298	10.599	39.063	1.00 36.34	A
ATOM	-			39.617	16.471	38.165	1.00 13.81	A
	1752	O.	LYS A 245	39.580	17.431	38.932	1.00 10.66	A
MOTA	1753	N	SER A 246	40.022	16.572	36.902	1.00 14.72	A
MOTA	1754	CA	SER A 246	40.405	17.856	36.344	1.00 11.87	A
ATOM	1755	CB	SER A 246	41.299	17.687	35.104	1.00 12.31	Α
MOTA	1756	OG	SER A 246	40.515	17.215	34.011	1.00 9.67	A
ATOM	1757	С	SER A 246	39.095	18.500	35.913	1.00 10.79	A
ATOM	1758	0	SER A 246	38.076	17.815	35.735	1.00 10.08	A
ATOM	1759	N	PRO A 247	39.114	19.825	35.698	1.00 10.98	A
ATOM	1760	CD	PRO A 247	40.243	20.747	35.947	1.00 7.03	A
ATOM	1761	CA	PRO A 247	37.909	20.545	35.275	1.00 9.29	Ä
MOTA	1762	CB	PRO A 247	38.210	21.988	35.692	1.00 7.19	Ä
ATOM	1763	CG	PRO A 247	39.737	22.094	35.385	1.00 7.13	
ATOM	1764	Č	PRO A 247	37.632	20.416	33.765		A
ATOM	1765	ŏ	PRO A 247					A
ATOM	1766	Ŋ	ALA A 248	36.865	21.197	33.222	1.00 11.54	A
ATOM	1767	CA	ALA A 248	38.253	19.449	33.083	1.00 9.23	A
ATOM	1768		ALA A 248	37.992	19.278	31.638	1.00 12.63	A
		СВ		38.832	18.097	31.069	1.00 10.35	A
ATOM ATOM	1769	C	ALA A 248	36.487	19.021	31.431	1.00 15.07	A
	1770	Ö.	ALA A 248	35.838	18.390	32.278	1.00 11.60	A
ATOM	1771	N	ALA A 249	35.935	19.497	30.311	1.00 12.95	A
MOTA	1772	CA	ALA A 249	34.498	19.332	30.037	1.00 11.90	A
ATOM	1773	CB	ALA A 249	34.141	19.886	28.633	1.00 12.61	A
MOTA	1774	Ç	ALA A 249	34.037	17.890	30.149	1.00 15.30	A
ATOM	1775	0	ALA A 249	32.953	17.617	30.666	1.00 14.63	A
ATOM	1776	N	ALA A 250	34.845	16.949	29.672	1.00 14.76	A
ATOM	1777	CA	ALA A 250	34.426	15.542	29.769	1.00 18.41	A
ATOM	1778	CB	ALA A 250	35.486	14.623	29.168	1.00 15.53	A
MOTA	1779	С	ALA A 250	34.118	15.102	31.200	1.00 15.76	A
ATOM ·	1780	0	ALA A 250	33.366	14.154	31.410	1.00 14.59	Ä
ATOM	1781	N	ASN A 251	34.677	15.785	32.190	1.00 14.82	A
ATOM	1782	CA	ASN A 251	34.433	15.380	33.575	1.00 13.85	Ä
ATOM	1783	CB	ASN A 251	35.665	15.696	34.441	1.00 12.26	Ä
ATOM	1784	ĊĠ	ASN A 251	36.880	14.885	34.022	1.00 14.85	Ã
ATOM	1785	OD1	ASN A 251	36.755	13.712	33.653	1.00 14.23	Â
ATOM	1786	ND2	ASN A 251	38.056	15.487	34.091	1.00 13.09	A
ATOM	1787	C	ASN A 251	33.168	15.968	34.210		
ATOM	1788	ŏ	ASN A 251	32.877	15.686	35.357	1.00 16.10	A
ATOM	1789	Ŋ	SER A 252				1.00 14.41	A
ATOM	1790	CA	SER A 252	32.431 31.191	16.806	33.482	1.00 13.25	Ā
ATOM	1791				17.346	34.039	1.00 10.81	A
		CB	SER A 252	31.262	18.868	34.209	1.00 22.32	A
ATOM	1792	og	SER A 252	31.266	19.536	32.953	1.00 23.58	Ā
ATOM	1793	Č	SER A 252	30.027	16.982	33.101	1.00 11.68	Ā
ATOM	1794	0	SER A 252	28.862	17.077	33.479	1.00 12.18	A
ATOM	1795	N	SER A 253	30.365	16.501	31.904	1.00 11.74	A
ATOM	1796	CA	SER A 253	29.367	16.138	30.918	1.00 10.64	A
ATOM	1797	СВ	SER A 253	30.048	15.572	29.665	1.00 18.81	A
ATOM	1798	og .	SER A 253	29.052	15.263	28.704	1.00 27.87	A
ATOM	1799	C	SER A 253	28.294	15.139	31.382	1.00 15.51	A
ATOM	1800	0	SER A 253	27.112	15.319	31.102	1.00 11.29	A
MOTA	1801	N	ALA A 254	28.692	14.080	32.081	1.00 12.85	A
ATOM	1802	CA	ALA A 254	27.700	13.084	32.525	1.00 14.75	A
ATOM	1803	CB	ALA A 254	28.423	11.868	33.216	1.00 13.94	A
ATOM	1804	C	ALA A 254	26.656	13.667	33.472	1.00 14.13	A
ATOM	1805	0	ALA A 254	25.457	13.394	33.342	1.00 14.40	A
MOTA	1806	N	ALA A 255	27.111	14.457	34.441	1.00 11.77	A
ATOM	1807	CA	ALA A 255	26.205	15.070	35.401	1.00 13.30	A
ATOM	1808	CB	ALA A 255	27.009	15.838	36.460	1.00 12.60	Ä
ATOM	1809	č	ALA A 255	25.223	16.017	34.698	1.00 15.34	Ä
ATOM	1810	ŏ	ALA A 255	24.068	16.162	35.113	1.00 14.03	À
ATOM	1811	N	ILE A 256	25.684	16.680	33.644	1.00 14.03	A
ATOM	1812	CA	ILE A 256	24.812				
					17.599	32.920	1.00 14.09	A
MOTA	1813	CB	ILE A 256	25.614	18.445	31.900	1.00 11.60	A
ATOM	1814	CG2	ILE A 256	24.655	19.233	30.987	1.00 13.12	A
MOTA	1815	CG1	ILE A 256	26.577	19.378	32.657	1.00 8.87	A
ATOM	1816	CD1	ILE A 256	25.878	20.335	33.703	1.00 6.00	A
MOTA	1817	Ç	ILE A 256	23.716	16.813	32.195	1.00 12.88	A
MOTA	1818	0	ILE A 256	22.569	17.268	32.118	1.00 12.14	A
MOTA	1819	N	SER A 257	24.069	15.639	31.678	1.00 12.01	A

MOTA	1896	CA	GLY A	268	6.491	30.653	30.439	1.00 13	રંગ ર	A
ATOM	1897	С	GLY A		7.212	31.457	31.507		3.92	Ä
ATOM	1898	0	GLY A		7.219	32.679	31.452		1.39	
ATOM	1899	N			7.804	30.767				A
ATOM	1900	CA	ASP A		8.554		32.486		1.00	A
ATOM	1901	CB	ASP A			31.398	33.594		4.58	A
					8.233	30.665	34.914		3.17	Α
ATOM	1902	CG	ASP A		8.943	31.263	36.117	1.00 16	5.24	A
MOTA	1903	OD1	ASP A	269	9.767	32.179	35.944	1.00 17	7.40	A
ATOM	1904	OD2	ASP A		8.667	30.804	37.244	1.00 19	9.44	A
MOTA	1905	С	ASP A	269	10.064	31.290	33.303	1.00 10		A
ATOM	1906	0	ASP A	269	10.616	30.196	33.348		1.39	A
ATOM	1907	N	PRO A		10.742	32.417	33.010		1.52	A
ATOM	1908	CD	PRO A		10.217	33.796	32.924	1.00 11		
ATOM	1909	CA	PRO A		12.184	32.394	32.709			A
ATOM	1910	CB	PRO A		12.523				0.44	A
ATOM	1911	CG	PRO A			33.867	32.491		L.04	A
ATOM					11.225	34.465	32.026	1.00 13		A
	1912	C	PRO A		13.042	31.786	33.793		2.77	A
ATOM	1913	O.	PRO A		14.097	31.243	33.521		0.58	A
ATOM	1914	N	ASN A		12.578	31.870	35.032	1.00 11	L.41	A
ATOM	1915	CA	ASN A		13.337	31.332	36.145	1.00 11	l.19	A
ATOM	1916	CB	ASN A	271	12.660	31.729	37.463	1.00 14	1.43	A
ATOM	1917	CG	ASN A	271	13.533	31.434	38.683	1.00 22		À
ATOM	1918	OD1	ASN A	271	14.734	31.726	38.696		5.89	A
ATOM	1919	ND2	ASN A	271	12.934	30.854	39.703		5.43	A
ATOM	1920	С	ASN A		13.545	29.816	36.090		5.21	Ä
MOTA	1921	Ō	ASN A		14.595	29.319	36.510		5.74	
ATOM	1922	Ň	VAL A		12.574	29.065				A
ATOM	1923	CA	VAL A				35.575		0.21	A
ATOM	1924	CB	VAL A		12.749	27.613	35.547		L.32	A
ATOM	1925				11.378	26.849	35.440		3.38	A
		CG1	VAL A		10.450	27.297	36.548		1.31	A
ATOM	1926	CG2	VAL A		10.759	27.074	34.078		L.03	A
ATOM	1927	Č	VAL A		13.651	27.086	34.434	1.00 12	2.71	A
ATOM	1928	0	VAL A		14.028	25.907	34.459	1.00 10	0.89	· A
ATOM	1929	N	TRP A		13.991	27.930	33.461	1.00 7	7.57	A
ATOM	1930	CA	TRP A	273	14.862	27.465	32.366	1.00 7	7.83	A
ATOM	1931	CB	TRP A	273	14.741	28.403	31.150		7.08	A
ATOM	1932	CG	TRP A	273	13.496	28.126	30.364		0.87	A
ATOM	1933	CD2	TRP A		13.359	27.161	29.325		9.80	Ä
ATOM	1934	CE2	TRP A		12.020	27.228	28.860		9.21	Â
ATOM	1935	CE3		273	14.241	26.240	28.732			
ATOM	1936	CD1	TRP A		12.271				7.74	A
ATOM	1937	NE1				28.728	30.500		7.74	A
ATOM				273	11.375	28.192	29.590		2.31	A
	1938	CZ2		273	11.545	26.412	27.838).97	A
ATOM	1939	CZ3	TRP A		13.764	25.428	27.700).91	A
MOTA	1940	CH2	TRP A		12.427	25.522	27.267	1.00 14	1.13	A
MOTA	1941	Ç	TRP A		16.338	27.311	32.755		9.26	A
MOTA	1942	0	TRP A		17.119	26.663	32.042	1.00 9	9.73	A
ATOM	1943	N	THR A		16.736	27.893	33.880	1.00 8	3.74	A
MOTA	1944	CA	THR A		18.123	27.769	34.281	1.00 11	l.71	A
ATOM	1945	CB	THR A	274	18.759	29.147	34.542	1.00 12	2.87	A
ATOM	1946	OG1	THR A	274	18.701	29.940	33.334	1.00 16	5.61	Α
MOTA	1947	CG2	THR A	274	20.240	28.973	34.959		9.96	A
MOTA	1948	С	THR A	274	18.271	26.918	35.535).53	Ä
ATOM	1949	0	THR A	274	18.020	27.378	36.645	1.00 11		A
ATOM	1950	N	PRO A		18.673	25.657	35.373	1.00 11		Ä
ATOM	1951	CD	PRO A		18.885	24.916	34.119	1.00 13		Â
ATOM	1952	CA	PRO A		18.841	24.782	36.543	1.00 11		
ATOM	1953	CB	PRO A		19.180	23.424	35.921			A
ATOM	1954	CG	PRO A			23.506	33.921	1.00 15		A
ATOM	1955	C			18.600		34.528		5.39	Ā
	1956	_	PRO A		20.004	25.253	37.445		.51	A
ATOM		O.	PRO A		21.007	25.723	36.950		.15	Ā
ATOM	1957	N	VAL A		19.869	25.148	38.764		9.91	A
ATOM	1958	CA	VAL A		20.999	25.502	39.615	1.00 10	0.08	A
ATOM	1959	СВ	VAL A		20.738	26.762	40.478	1.00 15	5.02	A
MOTA	1960	CG1	VAL A		20.534	27.990	39.568	1.00 16	5.57	A
ATOM	1961	CG2	VAL A	276	19.551	26.543	41.388	1.00 17		A
ATOM	1962	С	VAL A		21.236	24.293	40.500	1.00 12		A
ATOM	1963	0	VAL A		20.315	23.498	40.743		.21	A
ATOM	1964	Ň	PHE A		22.472	24.149	40.969		.38	Â
ATOM	1965	CA	PHE A		22.848	23.017	41.798		2.43	Â
ATOM	1966	CB	PHE A		24.231	22.491	41.373		1.49	Ä
ATOM	1967	CG	PHE A		24.229	21.828	40.017		1.19	
ATOM	1968			277	24.229					A
						22.568	38.858		7.76	A
ATOM	1969			277	23.999	20.461	39.909		1.15	A
MOTA	1970		PHE A		24.350	21.934	37.585		.41	Ā
MOTA	1971	CE2	PHE A	211	23.938	19.825	38.654	1.00 13	. 62	A

ATOM 1972 CZ PHE A 277			~-				27 400		
ATOM 1976 CA GLY A 278 22.892 24.553 43.634 1.00 12.80 A ATOM 1976 CA GLY A 278 22.767 22.602 45.540 1.00 12.01 A ATOM 1976 CA GLY A 278 22.767 22.602 45.540 1.00 12.01 A ATOM 1976 CA GLY A 278 22.767 22.602 45.540 1.00 12.01 A ATOM 1976 CA GLY A 278 22.767 22.602 45.540 1.00 12.01 A ATOM 1977 CO GLY A 278 22.767 22.602 45.540 1.00 12.01 A ATOM 1978 CA GLY A 278 22.1087 21.414 47.637 1.00 11.15 A ATOM 1980 CA ALA A 279 22.1087 21.414 47.637 1.00 11.15 A ATOM 1980 CA ALA A 279 22.1087 21.414 47.637 1.00 11.15 A ATOM 1981 CB ALA A 279 22.1087 21.414 47.637 1.00 11.15 A ATOM 1981 CB ALA A 279 22.1062 10.024 48.450 1.00 14.32 A ATOM 1981 CB ALA A 279 22.1062 10.024 48.450 1.00 14.32 A ATOM 1981 CB ALA A 279 22.1062 10.024 48.450 1.00 14.32 A ATOM 1981 CB ALA A 279 22.1062 10.024 48.450 1.00 14.32 A ATOM 1981 CB ALA A 279 22.1062 10.024 48.450 1.00 14.32 A ATOM 1984 N ALA A 280 22.20 18.176 47.796 1.00 18.01 A ATOM 1986 CB VAL A 280 19.500 17.847 49.076 1.00 19.81 A ATOM 1986 CC VAL A 280 19.500 17.847 49.076 1.00 19.81 A ATOM 1986 CC VAL A 280 19.500 17.847 49.076 1.00 19.81 A ATOM 1989 CC VAL A 280 19.01 11.848 18.82 46.686 1.00 20.63 A ATOM 1991 N THR A 281 18.812 17.436 46.055 1.00 21.63 A ATOM 1999 O VAL A 280 19.014 19.635 64.407 1.00 21.63 A ATOM 1999 C CT THR A 281 18.812 17.436 46.055 1.00 21.63 A ATOM 1999 C CT THR A 281 18.812 17.436 46.055 1.00 21.63 A ATOM 1999 C CT THR A 281 18.812 17.436 46.055 1.00 21.63 A ATOM 1999 C CT THR A 281 18.629 17.597 50.02 18.100 19.32 CB THR A 281 18.629 17.599 44.982 1.00 21.63 A ATOM 1999 C CT THR A 281 18.629 17.599 50.00 19.32 A ATOM 1999 C CT THR A 281 16.630 17.882 45.618 1.00 24.45 A ATOM 1999 C CT THR A 281 16.630 17.882 45.618 1.00 24.45 A ATOM 1999 C CT THR A 281 16.630 17.582 45.618 1.00 24.45 A ATOM 1999 C CT THR A 281 16.630 17.582 45.618 1.00 24.45 A ATOM 1999 C CT THR A 281 16.630 17.582 45.618 1.00 24.45 A ATOM 1999 C CT THR A 281 16.630 17.582 45.618 1.00 24.45 A ATOM 1999 C CT THR A 288 16.698 10.00 17.882 45.618 1.00 22.56 A ATOM 1999 C CT THR A 288 19.									
ATOM 1975 N GLY A 278 22.761 22.356 44.116 1.00 12.01 A ATOM 1976 CA GLY A 278 22.767 22.601 45.547 1.00 10.29 A ATOM 1977 C GLY A 278 23.113 21.342 46.303 1.00 10.29 A ATOM 1977 C GLY A 278 23.113 21.342 46.303 1.00 10.29 A ATOM 1977 C GLY A 278 23.113 21.342 46.303 1.00 10.29 A ATOM 1979 C N GLY A 278 23.103 21.304 47.7697 1.00 11.15 A ATOM 1979 C N GLY A 278 23.103 21.304 47.7697 1.00 11.15 A ATOM 1980 CA ALA A 279 23.602 20.604 48.450 1.00 14.32 A ATOM 1981 CB ALA A 279 23.62 C.604 49.930 1.00 16.91 A ATOM 1982 C ALA A 279 23.62 C.604 49.930 1.00 16.91 A ATOM 1982 C ALA A 279 23.62 C.604 49.930 1.00 16.91 A ATOM 1982 C ALA A 279 23.62 C.604 49.930 1.00 18.69 A ATOM 1982 C ALA A 279 23.62 C.604 49.930 1.00 18.69 A ATOM 1985 C ALA A 2800 20.302 118.102 44.70 10.01 18.69 A ATOM 1985 C ALA A 2800 20.302 118.102 47.796 1.00 19.81 A ATOM 1987 CGI VAL A 2800 20.457 17.579 50.225 1.00 23.28 A ATOM 1987 CGI VAL A 280 19.500 17.847 49.076 1.00 23.28 A ATOM 1988 CGZ VAL A 280 19.500 17.847 49.076 1.00 23.28 A ATOM 1989 C CA THR A 281 17.336 48.668 1.00 21.63 A ATOM 1999 C ATOM	-								
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NTOM 1979 N ALA 279 23.087 20.302 45.704 1.00 12.45 ALA ALA 279 23.087 21.414 47.637 1.00 11.15 ALA ALA ALA 279 23.087 21.414 47.637 1.00 11.15 ALA ALA ALA ALA 279 23.087 21.414 47.637 1.00 14.32 ALA ALA ALA ALA ALA 279 23.082 20.604 48.450 1.00 16.91 ALA								1.00 10.29	
ATOM 1998 CA LA A 2799 23.087 21.414 47.637 1.00 11.15 A ATOM 1980 CA LA A 2799 23.087 21.414 47.637 1.00 11.15 A ATOM 1980 CA LA A 2799 23.086 20.246 48.450 1.00 14.32 A ATOM 1981 CB ALA A 2799 22.542 19.029 48.157 1.00 18.91 A ATOM 1982 C ALA A 2799 22.542 19.029 48.157 1.00 18.91 A ATOM 1983 C ALA A 2799 22.542 19.029 48.157 1.00 18.91 A ATOM 1984 N NAL A 220 21.238 19.262 48.167 1.00 19.81 A ATOM 1986 CB VAL A 220 20.032 18.176 47.796 1.00 23.28 A ATOM 1986 CB VAL A 280 19.500 17.847 49.076 1.00 19.81 A ATOM 1986 CG VAL A 280 19.500 17.847 49.076 1.00 23.28 A ATOM 1988 CG2 VAL A 280 20.032 18.176 47.796 1.00 23.28 A ATOM 1988 CG2 VAL A 280 19.500 17.847 49.076 1.00 23.28 A ATOM 1988 CG2 VAL A 280 19.500 17.847 49.076 1.00 23.28 A ATOM 1988 CG2 VAL A 280 19.500 17.847 49.076 1.00 23.18 A ATOM 1998 C TAL A 280 19.500 17.847 49.076 1.00 23.18 A ATOM 1998 CG2 THR A 281 17.332 18.603 18.8992 49.436 1.00 21.63 A ATOM 1999 CA THR A 281 17.332 16.277 44.136 1.00 20.03 A ATOM 1991 N THR A 281 17.332 16.327 44.136 1.00 20.03 A ATOM 1993 CG THR A 281 17.332 16.327 44.136 1.00 20.03 A ATOM 1995 CG2 THR A 281 17.332 16.327 44.136 1.00 20.03 A ATOM 1995 CG2 THR A 281 18.899 16.096 41.493 1.00 20.20.70 A ATOM 1995 CG2 THR A 281 18.899 16.096 41.493 1.00 20.20.50 A ATOM 1995 CG2 THR A 281 18.899 16.096 41.493 1.00 20.20.50 A ATOM 1995 CG2 THR A 281 18.803 17.599 44.982 1.00 19.32 A ATOM 1995 CG2 THR A 281 18.803 1.073 17.159 46.520 1.00 20.20.56 A ATOM 1995 CG2 THR A 281 18.803 1.073 17.159 46.520 1.00 20.20.56 A ATOM 1995 CG CG2 THR A 281 18.803 1.073 17.159 46.520 1.00 20.20.56 A ATOM 1995 CG CG2 THR A 281 18.803 1.073 17.159 46.520 1.00 20.20.56 A ATOM 1995 CG CG2 THR A 281 18.803 1.073 17.159 46.520 1.00 20.20.56 A ATOM 2000 C GLY A 282 11.803 20.775 45.303 1.00 20.20.56 A ATOM 2000 C GLY A 282 11.803 20.775 45.303 1.00 20.20.56 A ATOM 2000 C GLY A 282 11.803 20.775 45.403 1.00 20.20.56 A ATOM 2000 C GLY A 282 11.803 20.775 45.403 1.00 20.20.56 A ATOM 2000 C GLY A 282 11.00 19.20 40.50 1.00 20.20 1.00 19.85 A ATOM 2000	MOTA								
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ATOM 2046 C PRO A 289 28.366 14.644 42.439 1.00 17.46 A									
ATOM 2010 C 100 100 100 15 200 A									A
								1.00 15.29	A

FIGURE 5 (suite)

MOTA	2048	N	ASP A 290	28.149	13.372	42.782	1.00 16.57	A
MOTA	2049	CA	ASP A 290	29.092	12.691	43.652	1.00 20.97	A
MOTA	2050	CB	ASP A 290	28.360	11.751	44.628	1.00 25.52	A
MOTA	2051	CG	ASP A 290	27.489	10.723	43.929	1.00 34.64	A
MOTA	2052	OD1		26.599	10.146	44.604	1.00 38.07	Α
ATOM	2053	OD2		27.693	10.478	42.716	1.00 39.24	A
MOTA	2054	C	ASP A 290	30.154	11.952	42.824	1.00 21.23	A
ATOM	2055	0	ASP A 290	30.990	11.231	43.362	1.00 21.11	A
ATOM	2056	N	SER A 291	30.136	12.152	41.509	1.00 14.24	A
ATOM	2057	CA	SER A 291	31.143	11.538	40.645	1.00 16.28	A
ATOM	2058	CB	SER A 291	30.592	10.290	39.925	1.00 16.14	Ā
ATOM	2059	og .	SER A 291	29.549	10.625	39.031	1.00 22.17	A
ATOM	2060	C	SER A 291	31.555	12.609	39.643	1.00 14.75	A
MOTA MOTA	2061 2062	O N	SER A 291	30.842	13.605	39.493	1.00 13.50	A
ATOM	2062	CA	GLY A 292 GLY A 292	32.692 33.181	12.419 13.423	38.971 38.019	1.00 13.79 1.00 14.60	A A
ATOM	2064	c	GLY A 292	33.713	14.688	38.707	1.00 14.00	A
ATOM	2065	ŏ	GLY A 292	33.964	14.669	39.909	1.00 14.10	Ä
ATOM	2066	Ň	TYR A 293	33.904	15.779	37.955	1.00 10.56	Ã
MOTA	2067	CA	TYR A 293	34.380	17.049	38.529	1.00 9.23	Ä
ATOM	2068	CB	TYR A 293	34.838	18.014	37.443	1.00 10.30	A
ATOM	2069	CG	TYR A 293	35.535	19.229	38.012	1.00 11.13	A
ATOM	2070	CD1	TYR A 293	36.829	19.138	38.526	1.00 7.85	A
ATOM	2071	CE1	TYR A 293	37.482	20.269	39.049	1.00 8.64	А
ATOM	2072	CD2	TYR A 293	34.900	20.470	38.038	1.00 11.82	A
MOTA	2073	CE2	TYR A 293	35.547	21.601	38.554	1.00 11.43	A
ATOM	2074	CZ	TYR A 293	36.839	21.488	39.052	1.00 8.40	A
ATOM	2075	ОН	TYR A 293	37.488	22.625	39.496	1.00 8.49	A
ATOM	2076	C	TYR A 293	33.183	17.645	39.252	1.00 9.71	A
ATOM	2077	0	TYR A 293	32.142	17.834	38.657	1.00 12.02	Ä
ATOM	2078 2079	И	PRO A 294	33.347	18.021	40.531	1.00 12.25 1.00 12.44	A
MOTA MOTA	2079	CD CA	PRO A 294 PRO A 294	34.575 32.229	17.923 18.559	41.350 41.302	1.00 12.44 1.00 14.24	A A
ATOM	2081	CB	PRO A 294	32.644	18.263	42.748	1.00 14.24	Ä
ATOM	2082	CG	PRO A 294	34.132	18.499	42.712	1.00 15.49	Ā
ATOM	2083	č	PRO A 294	31.682	19.963	41.133	1.00 13.85	Ä
ATOM	2084	ŏ	PRO A 294	30.511	20.171	41.429	1.00 11.37	Ä
MOTA	2085	N	ILE A 295	32.476	20.907	40.628	1.00 10.88	A
ATOM	2086	CA	ILE A 295	31.990	22.280	40.510	1.00 9.12	A
MOTA	2087	CB	ILE A 295	33.062	23.301	40.934	1.00 10.07	A
ATOM	2088	CG2	ILE A 295	32.375	24.666	41.232	1.00 10.52	A
ATOM	2089	CG1	ILE A 295	33.733	22.853	42.236	1.00 12.06	A
ATOM	2090	CD1		34.841	23.801	42.703	1.00 12.46	A
ATOM	2091	Ċ	ILE A 295	31.564	22.574	39.087	1.00 12.87	A
MOTA	2092	0	ILE A 295	32.397	22.660	38.182	1.00 10.57	A
ATOM ATOM	2093 2094	N	LEU A 296 LEU A 296	30.257 29.703	22.743 22.951	38.902 37.570	1.00 10.82 1.00 8.61	A A
ATOM	2095	CA CB	LEU A 296	29.370	21.578	36.949	1.00 9.63	A
ATOM	2096	ĊĞ	LEU A 296	28.032	20.884	37.276	1.00 7.75	A
ATOM	2097	CD1		27.971	19.517	36.572	1.00 11.60	Ä
ATOM	2098	CD2		27.852	20.690	38.784	1.00 10.20	A
ATOM	2099	C	LEU A 296	28.461	23.828	37.612	1.00 7.00	A
ATOM	2100	0	LEU A 296	27.945	24.137	38.690	1.00 11.47	A
ATOM	2101	N	GLY A 297	27.988	24.236	36.436	1.00 8.98	A
ATOM	2102	CA	GLY A 297	26.812	25.093	36.353	1.00 8.75	A
ATOM	2103	Ç	GLY A 297	26.503	25.452	34.906	1.00 14.03	A
ATOM	2104	0	GLY A 297	27.128	24.917	33.979	1.00 9.23	A
ATOM	2105	N	PHE A 298	25.544	26.353	34.700	1.00 7.40	A
MOTA	2106	CA	PHE A 298	25.177	26.758	33.350 33.105	1.00 7.84	A
ATOM	2107 2108	CB CG	PHE A 298 PHE A 298	23.666 23.249	26.550 25.102	32.984	1.00 6.30	A A
MOTA MOTA	2108		PHE A 298 PHE A 298	22.775	24.398	34.094	1.00 10.10	Ã
ATOM	2110	CD2		23.356	24.444	31.763	1.00 8.37	Ā
MOTA	2111	CE1		22.414	23.038	33.988	1.00 13.84	Â
MOTA	2112	CE2		23.005	23.087	31.630	1.00 7.19	A
ATOM	2113	CZ	PHE A 298	22.533	22.379	32.747	1.00 12.00	A
ATOM	2114	č	PHE A 298	25,469	28.235	33.145	1.00 10.22	A
ATOM	2115	Ō	PHE A 298	25.431	29.007	34.114	1.00 9.27	A
ATOM	2116	N	THR A 299	25.811	28.615	31.910	1.00 7.04	A
ATOM	2117	CA	THR A 299	25.961	30.029	31.594	1.00 8.99	Ā
MOTA	2118	CB	THR A 299	27.319	30.414	30.975	1.00 12.65	A
ATOM	2119	OG1		27.293	31.818	30.682	1.00 10.67	A
ATOM	2120	CG2		27.616	29.617	29.740	1.00 12.18	A
ATOM	2121	C	THR A 299	24.798	30.220	30.616	1.00 8.12 1.00 9.48	A A
MOTA	2122	O N	THR A 299	24.482 24.173	29.325 31.392	29.810 30.677	1.00 9.48 1.00 8.49	A
MOTA	2123	N	00E A 92A	64.1/3	31.336	30.677	1.00 0.49	^

ATOM	2124	CA	ASP A	300	22.930	31.636	29.950	1.00 10.66	A
MOTA MOTA	2125 2126	CB CG	ASP A		21.849	31.816	31.023	1.00 8.23	A
ATOM	2127		ASP A		22.055 22.141	30.877 29.660	32.193 31.928	1.00 14.11 1.00 8.23	A A
MOTA	2128	OD2	ASP A		22.149	31.341	33.373	1.00 15.65	Ä
ATOM ATOM	2129 2130	C O	ASP A		22.828 23.690	32.790	28.975	1.00 10.65	A
ATOM	2131	Ň	LEU A		21.740	33.669 32.765	28.931 28.202	1.00 8.49 1.00 8.77	A A
ATOM	2132	CA	LEU A		21.407	33.819	27.246	1.00 10.49	A
MOTA MOTA	2133 2134	CB CG	LEU A		21.121 22.189	33.226 32.371	25.850 25.157	1.00 10.57	A
MOTA	2135	CD1	LEU A	301	21.699	31.951	23.775	1.00 17.61 1.00 16.46	A A
MOTA MOTA	2136 2137		LEU A		23.456	33.151	25.057	1.00 12.96	A
ATOM	2138	C	LEU A		20.128 19.179	34.533 33.889	27.689 28.127	1.00 7.85 1.00 7.63	A A
MOTA	2139	N	ILE A		20.101	35.855	27.564	1.00 8.91	A
ATOM ATOM	2140 2141	CA CB	ILE A		18.897 19.146	36.614 37.648	27.879 29.000	1.00 7.82 1.00 10.36	A A
MOTA	2142	CG2	ILE A	302	17.848	38.429	29.261	1.00 10.30	A
ATOM ATOM	2143 2144	CG1 CD1	ILE A		19.588	36.918	30.287	1.00 8.81	A
ATOM	2145	C	ILE A		20.089 18.517	37.867 37.368	31.411 26.602	1.00 7.82 1.00 9.48	A A
ATOM	2146	0	ILE A	302	19.320	38.158	26.096	1.00 8.44	A
ATOM ATOM	2147 2148	N CA	PHE A		17.311 16.843	37.120 37.786	26.081 24.854	1.00 8.80 1.00 8.37	A A
MOTA	2149	СВ	PHE A	. 303	16.751	36.821	23.651	1.00 7.07	A
ATOM ATOM	2150 2151	CG CD1	PHE A		18.054 19.027	36.583	22.944	1.00 8.30	A
ATOM	2152	CD2	PHE A		18.316	35.770 37.205	23.500 21.725	1.00 8.48 1.00 7.08	A A
ATOM	2153	CE1	PHE A		20.265	35.582	22.851	1.00 7.30	A
ATOM ATOM	2154 2155	CE2 CZ	PHE A		19.559 20.528	37.023 36.210	21.065 21.637	1.00 9.28 1.00 11.64	A A
MOTA	2156	С	PHE A	303	15.437	38.305	25.032	1.00 9.03	Ä
ATOM ATOM	2157 2158	O N	PHE A		14.797 14.947	38.052	26.031	1.00 9.30	A
ATOM	2159	CA	SER A		13.566	39.002 39.465	24.014 24.044	1.00 7.56 1.00 9.72	A A
ATOM	2160	CB	SER A		13.470	40.870	23.444	1.00 11.08	A
ATOM ATOM	2161 2162	OG C	SER A		12.117 12.707	41.291 38.530	23.498 23.170	1.00 10.08 1.00 6.80	A A
MOTA	2163	ŏ	SER A		13.198	38.018	22.162	1.00 10.90	A
ATOM ATOM	2164 2165	N	GLU A		11.451	38.293	23.534	1.00 8.14	A
ATOM	2166	CA CB	GLU A		10.605 9.268	37.482 37.125	22.655 23.316	1.00 11.11 1.00 10.66	A A
MOTA	2167	CG	GLU A	305	8.447	36.161	22.439	1.00 11.71	A
ATOM ATOM	2168 2169	CD OE1	GLU A		7.073 6.767	35.820 36.154	22.985 24.147	1.00 12.77 1.00 14.12	A A
MOTA	2170	OE2	GLU A	305	6.288	35.192	22.228	1.00 16.70	Ä
ATOM ATOM	2171 2172	C O	GLU A		10.305 10.154	38.329 37.800	21.399 20.283	1.00 15.34 1.00 10.74	A
MOTA	2173	N	CYS A		10.239	39.649	21.574	1.00 10.74 1.00 11.86	A A
ATOM ATOM	2174 2175	CA	CYS A		9.889	40.534	20.450	1.00 12.96	A
ATOM	2176	C	CYS A	306	10.859 11.434	41.666 42.270	20.140 21.046	1.00 14.14 1.00 11.98	A A
ATOM	2177	CB		306	8.531	41.185	20.726	1.00 11.40	Α
ATOM ATOM	2178 2179	SG N	CYS A	306 307	7.188 11.017	40.111 41.956	21.313 18.854	1.00 15.63 1.00 12.82	A A
ATOM	2180.	CA	TYR A	307	11.872	43.060	18.397	1.00 10.85	Ä
ATOM ATOM	2181 2182	CB CG	TYR A		13.143 14.066	42.533 41.850	17.712	1.00 8.88	A
ATOM	2183	CD1	TYR A		13.902	40.499	18.703 19.020	1.00 13.96 1.00 13.44	A A
ATOM	2184	CEI	TYR A		14.683	39.882	20.020	1.00 13.43	Α
ATOM ATOM	2185 2186	CD2 CE2	TYR A		15.035 15.821	42.579 41.972	19.401 20.410	1.00 11.32 1.00 11.99	A A
MOTA	2187	CZ	TYR A	307	15.637	40.625	20.712	1.00 12.10	A
MOTA MOTA	2188 2189	С Он	TYR A		16.379 11.056	40.019 43.908	21.724 17.424	1.00 12.32	A
ATOM	2190	ŏ	TYR A		10.318	43.370	16.588	1.00 13.04 1.00 11.71	A A
ATOM	2191	N	ALA A		11.161	45.229	17.546	1.00 13.47	Α
ATOM ATOM	2192 2193	CA CB	ALA A		10.420 10.623	46.123 47.583	16.660 17.116	1.00 19.16 1.00 19.39	A A
MOTA	2194	C	ALA A	308	10.827	45.960	15.176	1.00 16.58	A
ATOM ATOM	2195 2196	O N	ALA A ASN A		9.990 12.109	46.011	14.290	1.00 15.94	A
ATOM	2197	CA	ASN A		12.621	45.752 45.602	14.919 13.565	1.00 16.56 1.00 15.71	A A
MOTA	2198	CB	ASN A	309	14.084	46.052	13.558	1.00 11.74	A
ATOM	2199	CG	ASN A	309	14.704	46.002	12.183	1.00 20.62	A

ATOM 2200 OD1 15.130 14.741 12.493 44.946 47.153 **ASN A 309** 11.713 11.517 13.066 1.00 17.26 1.00 13.84 ASN A 309 MOTA 2201 ND2 ATOM 2202 ASN A 309 44.142 1.00 16.39 ASN A MOTA 2203 0 309 13.031 43.221 13.678 1.00 11.54 A 2204 N CA CB ATOM ALA A 310 11.806 43.942 11.941 1.00 12.69 A 2205 MOTA ALA A 310 11.583 42.584 11.430 1.00 16.06 ATOM 2206 ALA A 310 ALA A 310 ALA A 310 10.564 42.618 10.281 1.00 16.44 ATOM 2207 12.836 41.828 40.599 10.997 1.00 14.76 MOTA 2208 12.907 11.128 1.00 15.90 THR A 311 THR A 311 10.485 ATOM 2209 N 13.827 42.546 1.00 13.61 1.00 14.28 MOTA 2210 CA 15.074 41.922 14.28 1.00 15.47 1.00 18.10 ATOM 2211 CB THR A 311 15.949 42.927 9.314 ATOM 2212 OG1 THR A 311 15.284 8.097 43.307 ATOM 2213 CG2 THR A 311 17.291 42.322 8.977 1.00 16.40 A 2214 ATOM THR A 311 15.813 41.407 11.324 1.00 15.00 THR A 311 THR A 311 GLN A 312 2215 MOTA Õ 16.371 15.798 16.477 11.318 40.313 1.00 12.29 ATOM 2216 N 42.180 41.717 12.409 1.00 13.08 MOTA 2217 CA 1.00 12.35 1.00 10.08 1.00 7.89 13.623 MOTA 2218 CB 14.682 16.545 42.827 MOTA 2219 ÇG 17.501 43.960 14.273 A MOTA 2220 CD 17.696 44.997 15.377 1.00 13.93 Α OE1 16.311 15.255 MOTA 2221 2222 **GLN A 312** 16.897 45.087 1.00 14.28 MOTA 18.743 15.768 NE₂ **GLN A 312** 45.799 1.00 16.18 ATOM 2223 **GLN A 312** co 40.486 14.191 1.00 11.19 2224 GLN A 312 THR A 313 THR A 313 1.00 14.09 1.00 9.72 1.00 8.88 1.00 13.95 1.00 14.46 MOTA 14.639 14.189 14.685 16.418 39.537 40.507 A ATOM 2225 N 14.439 13.670 CA CB ATOM 2226 39.363 A ATOM 2227 THR A 313 12.149 39.541 14.449 Α THR A 313 ATOM 2228 OG1 11.660 15.197 40.660 Α 2229 2230 2231 CG₂ ATOM THR A 313 11.398 38.288 14.882 1.00 THR A 313 THR A 313 ATOM CO 14.108 38.096 13.935 1.00 10.80 ATOM 14.318 37.042 14.538 1.00 11.41 2232 GLY A 314 GLY A 314 GLY A 314 1.00 11.55 1.00 12.96 1.00 10.31 1.00 11.80 MOTA 12.615 11.810 N 14.218 38.204 2233 CA 37.067 ATOM 14.628 A 12.090 12.111 12.291 16.060 16.370 2234 CO MOTA 1.00 10.31 1.00 11.80 1.00 10.00 36.638 Α ATOM 2235 **GLY A 314** 35.439 ATOM 2236 N **GLN A 315** 16.952 37.603 GLN A 315 GLN A 315 ATOM 2237 CA 18.360 37.280 12.586 1.00 10.98 12.512 11.071 ATOM 2238 CB 19.219 38.542 1.00 12.34 MOTA 2239 CG GLN A 315 19.286 39.069 1.00 13.86 2240 GLN A 315 GLN A 315 GLN A 315 **ATOM** CD 20.014 40.385 10.958 1.00 16.05 2241 OE1 ATOM 19.868 20.787 41.254 11.818 9.880 1.00 15.65 1.00 15.34 2242 **ATOM** NE2 40.552 A 1.00 11.33 1.00 12.86 1.00 11.99 2243 GLN A 315 18.518 13.952 14.136 **ATOM** 36.613 35.743 MOTA 2244 GLN A 315 19.385 VAL A 316 VAL A 316 MOTA 2245 N 17.677 37.006 14.909 CA CB MOTA 2246 17.719 36.389 16.238 1.00 11.29 VAL A 316 MOTA 2247 16.803 37.131 17.251 1.00 12.97 16.658 17.401 17.232 17.813 **ATOM** 2248 2249 CG1 CG2 1.00 12.95 1.00 11.75 36.292 18.541 MOTA 38.493 17.602 16.092 16.667 11.75 A MOTA 2250 č 34.929 1.00 13.11 1.00 12.64 1.00 9.04 ATOM 2251 0 33.996 A **ATOM** 2252 N **ARG A 317** 34.723 15.327 16.164 A CA CB 15.115 **ATOM** 2253 ARG A 317 15.672 33.364 1.00 12.87 A MOTA 2254 ARG A 317 14.348 33.372 14.303 1.00 14.06 2255 2256 2257 CG ATOM ARG A 317 13.148 33.951 15.076 1.00 13.07 ARG A 317 ARG A 317 ARG A 317 14.243 MOTA 11.823 33.964 1.00 14.93 ATOM NE 13.765 14.480 15.704 11.520 10.894 32.611 31.677 1.00 14.57 2258 MOTA CZ 1.00 10.03 1.00 9.62 A ARG A 317 ARG A 317 ATOM 2259 NH1 10.470 31.934 2260 MOTA NH2 10.730 30.461 13.983 1.00 13.56 16.730 16.879 14.434 14.783 MOTA 2261 ARG A 317 32.491 1.00 12.01 ATOM 2262 0 ARG A 317 31.320 1.00 12.09 2263 2264 ATOM N ASN A 318 17.462 33.033 13.464 1.00 11.68 A 12.796 11.629 ATOM CA CB A 318 A 318 ASN 18.503 32.246 1.00 13.18 2265 ATOM ASN 19.123 33.028 1.00 11.52 A 318 A 318 18.145 17.140 10.500 ASN 33.249 32.557 15.15 13.70 17.31 MOTA 2266 CG 1.00 2267 OD1 ATOM ASN MOTA 18.438 34.211 2268 ND2 ASN A 318 9.638 1.00 A ATOM 2269 ASN 19.613 31.841 1.00 12.19 MOTA 2270 0 ASN 318 20.207 30.753 13.658 1.00 9.01 ATOM 2271 N PHE A 319 19.904 32.715 14.733 1.00 10.68 20.936 21.274 9.90 ATOM 2272 CA PHE А 319 32.376 15.707 1.00 33.577 MOTA 2273 CB PHE A 319 16.584 17.794 1.00 7.66 PHE A 319 PHE A 319 MOTA 2274 CG 22.105 33.212 1.00 10.09 A 32.644 MOTA 2275 CD1 23.351 17.631 1.00 6.01

ATOM 2276 CD2 PHE A 319 21.593 33.356 19.087 1.00 10.54 2277 CE1 24.102 22.333 23.589 ATOM PHE A 319 18.738 32.203 1.00 12.72 1.00 15.07 A 2278 CE2 32.919 MOTA PHE A 319 20.212 MOTA 2279 CZPHE A 319 32.338 20.027 1.00 12.59 **ATOM** 2280 PHE A 319 20.449 31.222 16.587 1.00 10.27 MOTA 2281 O PHE A 319 21.203 30.282 16.868 1.00 12.47 MOTA 2282 N PHE A 320 19.188 17.013 31.275 1.00 10.21 ATOM 2283 CA CB PHE A 320 18.649 30.213 17.860 1.00 10.79 ATOM 2284 PHE A 320 17.247 30.581 18.363 1.00 9.11 **ATOM** 2285 PHE A 320 1.00 CG 17.246 31.285 19.698 7.96 16.762 MOTA 2286 CD1 PHE A 320 30.642 20.833 1.00 9.52 PHE 17.723 16.750 **ATOM** 2287 CD2 A 320 32.583 19.822 1.00 12.60 ATOM 2288 CE1 PHE A 320 31.282 22.082 1.00 6.69 MOTA 2289 CE2 PHE A 320 17.712 33.244 21.075 1.00 9.45 ATOM 2290 CZPHE A 320 17.220 32.579 22.209 1.00 8.89 2291 ATOM PHE A 320 18.598 28.912 17.089 1.00 7.76 ATOM 2292 0 PHE A 320 18.856 27.838 17.634 9.90 1.00 2293 ATOM N THR A 321 18.274 29.013 15.801 1.00 8.04 CA THR A 321 27.829 ATOM 2294 18.199 14.950 1.00 6.79 A 2295 MOTA 28.224 13.551 CB THR A 321 17.687 1.00 7.01 **ATOM** 2296 OG1 THR A 321 16.334 28.695 13.691 1.00 11.25 2297 MOTA CG2 THR A 321 17.731 27.032 12.573 1.00 9.32 MOTA 2298 THR A 321 19.535 27.128 14.872 1.00 11.09 Α MOTA 2299 0 THR A 321 19.594 25.896 14.823 1.00 10.46 Α MOTA 2300 N LYS A 322 20.617 27.904 14.873 1.00 8.41 Α MOTA 2301 CA LYS A 322 21.950 27.319 14.849 1.00 8.00 A MOTA 2302 CB LYS A 322 22.970 28.329 14.299 1.00 6.38 A MOTA 2303 CG LYS A 322 24.410 27.805 14.359 1.00 10.15 A MOTA 2304 CD LYS A 322 25.396 28.712 13.615 1.00 8.08 Α MOTA 2305 CE LYS A 322 26.665 27.922 13.317 1.00 11.78 A MOTA NZ LYS A 322 2306 27.577 28.702 12.437 1.00 18.79 Α MOTA 322 26.857 16.242 2307 LYS Α 22.415 1.00 9.52 Α 2308 MOTA LYS A 322 22.864 25.711 27.735 16.425 1.00 9.02 A ATOM 2309 HIS 323 22.289 17.231 Α 10.06 1.00 Α 2310 CA HIS A 323 18.569 MOTA 22.793 27.420 9.00 1.00 A MOTA 2311 CB HIS A 323 22.710 7.78 28.677 19.469 1.00 A 20.637 HIS A 323 23.655 9.56 MOTA 2312 CG 28.657 1.00 A MOTA 2313 CD2 HIS A 323 23.426 28.762 1.00 9.53 Α 25.028 25.602 MOTA 2314 ND1 HIS A 323 28.560 20.494 1.00 7.88 A HIS A 323 HIS A 323 MOTA 2315 CE1 28.615 21.683 1.00 9.47 A NE2 MOTA 2316 24.653 28.736 22.598 1.00 12.97 A 2317 HIS A 323 MOTA C 22.082 26.230 19.222 1.00 9.52 A MOTA 2318 0 HIS A 323 22.687 25.507 20.019 1.00 8.65 MOTA 2319 N **TYR A 324** 20.808 26.034 18.877 1.00 9.61 **TYR A 324** 1.00 10.38 MOTA 2320 CA 20.024 24.911 19.427 CB 6.95 MOTA 2321 TYR A 324 18.767 25.434 20.149 1.00 26.376 27.752 1.00 MOTA 2322 CG TYR A 324 19.137 21.277 7.33 MOTA 2323 CD1 **TYR A 324** 19.195 21.072 5.99 1.00 8.99 ATOM 2324 CE1 TYR A 324 19.656 28.618 22.097 1.00 MOTA 2325 CD2 TYR A 324 19.533 25.882 22.513 1.00 7.61 Α MOTA 2326 CE2 TYR A 324 19.994 26.731 23.525 1.00 5.98 ATOM 2327 CZTYR A 324 20.052 28.094 23.303 1.00 7.54 OH 7.56 MOTA 2328 TYR A 324 20.547 28.926 24.294 1.00 MOTA 2329 TYR A 324 19.627 23.893 18.338 1.00 7.02 23.118 MOTA 2330 O **TYR A 324** 18.677 1.00 10.94 18.498 MOTA 2331 **GLY A 325** 20.387 23.868 17.254 7.94 N 1.00 2332 CA **GLY A 325** 20.064 22.938 7.51 MOTA 16.181 1.00 2333 **GLY A 325** 21.493 MOTA 20.514 16.386 1.00 12.01 Α 21.492 19.788 ATOM 2334 **GLY A 325** 21.227 17.097 1.00 10.59 THR A 326 THR A 326 ATOM 20.564 15.752 1.00 8.75 A 2336 CA 20.113 19.132 15.790 1.00 10.25 ATOM 15.135 15.708 ATOM 2337 CB THR A 326 19.005 18.311 1.00 9.46 A 2338 OG1 THR A 326 17.759 18.707 1.00 10.73 ATOM THR A 326 THR A 326 CG2 2339 19.212 16.788 15.369 **ATOM** 1.00 7.67 A 2340 18.937 15.038 **ATOM** 21.432 1.00 9.78 2341 THR A 326 15.452 **ATOM** 22.278 18.131 1.00 10.90 SER A 327 13.953 ATOM 2342 21.614 19.688 1.00 12.37 19.666 18.752 ATOM 2343 CA **SER A 327** 22.858 13.176 1.00 11.58 MOTA 2344 CB SER A 327 22.743 11.935 1.00 14.65 **ATOM** OG 19.192 1.00 2345 SER A 327 21.725 11.051 10.13 A 327 2346 C SER **ATOM** 23.158 21.118 12.764 1.00 10.87 A MOTA 2347 0 SER A 327 22.419 22.031 13.149 1.00 9.05 ATOM 2348 N ALA A 328 24.228 21.331 12.000 1.00 11.22 A ALA ATOM 2349 CA A 328 24.637 22.690 11.567 1.00 10.30 A 328 MOTA 2350 CB ALA А 23.682 23.234 10.518 1.00 12.01 A MOTA 2351 ALA A 328 24.602 23.592 12.790 1.00 11.88

ATOM	2352	0	ATA A 7	20	24 046				
			ALA A 3		24.046	24.674	12.742	1.00 13.69	Α
MOTA	2353	N	ASN A 3		25.197	23.140	13.887	1.00 11.26	A
ATOM	2354	CA	ASN A 3	29	25.150	23.910	15.123	1.00 10.51	A
ATOM	2355	CB	ASN A 3	29	24.422	23.083	16.205	1.00 8.81	
MOTA	2356	CG	ASN A 3		25.132	21.771	16.536	1.00 9.32	
ATOM	2357	OD1	ASN A 3		26.352				
ATOM	2358	ND2	ASN A 3			21.717	16.573	1.00 11.49	
ATOM					24.360	20.714	16.792	1.00 10.75	
	2359	C	ASN A 3		26.526	24.402	15.604	1.00 12.21	A
ATOM	2360	0	ASN A 3		27.515	24.381	14.849	1.00 9.35	A
ATOM	2361	N	ASP A 3	30	26.586	24.863	16.851	1.00 10.38	
ATOM	2362	CA	ASP A 3	30	27.837	25.386	17.412	1.00 9.41	
ATOM	2363	CB	ASP A 3	30	27.575	26.677	18.208	1.00 10.91	Ä
MOTA	2364	CG	ASP A 3		27.239	27.852	17.331		
MOTA	2365	OD1	ASP A 3		26.333			1.00 13.71	A
ATOM	2366	OD2	ASP A 3			28.653	17.720	1.00 14.93	· A
ATOM	2367				27.880	27.981	16.261	1.00 10.16	Α
		C	ASP A 3		28.536	24.416	18.346	1.00 10.31	A
ATOM	2368	0	ASP A 3		29.484	24.809	19.029	1.00 8.29	A
MOTA	2369	N	ASN A 3		28.111	23.153	18.363	1.00 8.79	A
MOTA	2370	CA	ASN A 3	31	28.698	22.217	19.311	1.00 10.91	A
ATOM	2371	CB	ASN A 3	31	27.942	20.869	19.267	1.00 11.40	
ATOM	2372	CG	ASN A 3	31	26.579	20.924	19.989	1.00 15.36	A
ATOM	2373	OD1	ASN A 3		25.926	19.893	20.194	1.00 12.09	
ATOM	2374	ND2	ASN A 3		26.156	22.115			
ATOM	2375	C	ASN A 3				20.372	1.00 9.71	Ā
					30.220	22.012	19.218	1.00 12.28	A
ATOM	2376	0	ASN A 3		30.877	21.866	20.255	1.00 12.57	A
ATOM	2377	N	ALA A 3		30.795	22.001	18.012	1.00 10.00	A
ATOM	2378	CA	ALA A 3		32.252	21.842	17.903	1.00 12.41	A
ATOM	2379	CB	ALA A 3		32.677	21.733	16.445	1.00 12.06	A
ATOM	2380	С	ALA A 3	32	32.964	23.028	18.548	1.00 8.53	A
MOTA	2381	0	ALA A 3	32	33.973	22.872	19.247	1.00 11.75	Ä
ATOM	2382	N	ALA A 3	33	32.447	24.216	18.297	1.00 9.64	A
ATOM	2383	CA	ALA A 3		33.057	25.422	18.858		
ATOM	2384	CB	ALA A 3					1.00 10.83	A
					32.424	26.655	18.223	1.00 9.42	A
ATOM	2385	Č	ALA A 3		32.910	25.473	20.379	1.00 10.44	A
ATOM	2386	0	ALA A 3		33.787	25.982	21.096	1.00 9.81	A
ATOM	2387	N	ILE A 3		31.787	24.963	20.869	1.00 9.49	Α
ATOM	2388	CA	ILE A 3	34	31.536	24.919	22.305	1.00 10.34	Α
ATOM	2389	CB	ILE A 3	34	30.099	24.404	22.567	1.00 7.35	A
ATOM	2390	CG2	ILE A 3	34	29.902	24.030	24.056	1.00 4.48	A
MOTA	2391	CG1	ILE A 3		29.093	25.467	22.091	1.00 8.68	A
ATOM	2392	CD1	ILE A 3		27.628	24.953	22.043	1.00 8.29	
ATOM	2393	C	ILE A 3						Ā
ATOM					32.593	24.003	22.946	1.00 9.03	A
	2394	Ö.	ILE A 3		33.239	24.352	23.954	1.00 6.82	A
ATOM	2395	N	GLN A 3		32.805	22.847	22.333	1.00 6.99	Α
MOTA	2396	CA	GLN A 3		33.800	21.903	22.831	1.00 8.99	A
MOTA	2397	CB	GLN A 3		33.695	20.589	22.053	1.00 11.58	Α
ATOM	2398	CG	GLN A 3	35	32.448	19.784	22.446	1.00 21.44	Α
ATOM	2399	CD	GLN A 3	35	32.279	18.518	21.598	1.00 30.71	A
MOTA	2400	OE1	GLN A 3	35	33.212	18.083	20.927	1.00 34.68	A
MOTA	2401	NE2	GLN A 3		31.089	17.926	21.638	1.00 37.34	A
ATOM	2402	C	GLN A 3		35.223	22.438	22.774		
ATOM	2403	ŏ	GLN A 3					1.00 12.27	A
ATOM	2404	Ŋ			36.014	22.219	23.704	1.00 10.25	Ā
MOTA			ALA A 3		35.547	23.143	21.690	1.00 10.75	Ā
	2405	CA	ALA A 3		36.868	23.726	21.514	1.00 12.71	A
ATOM	2406	CB	ALA A 3		36.989	24.375	20.091	1.00 9.35	A
ATOM	2407	C	ALA A 3		37.109	24.794	22.591	1.00 11.11	A
ATOM	2408	0	ALA A 3.		38.247	25.134	22.894	1.00 11.00	A
ATOM	2409	N	ASN A 3	37	36.025	25.310	23.164	1.00 8.06	A
ATOM	2410	CA	ASN A 3		36.125	26.342	24.185	1.00 9.10	A
ATOM	2411	CB	ASN A 3		35.098	27.440	23.887	1.00 8.86	Ä
MOTA	2412	ČĞ	ASN A 3		35.621	28.457	22.874	1.00 12.21	
ATOM	2413		ASN A 3		36.333				A
ATOM			ASN A 3			29.417	23.230	1.00 12.38	A
	2414	ND2			35.301	28.237	21.605	1.00 13.95	A
MOTA	2415	C	ASN A 3		35.979	25.816	25.622	1.00 9.52	A
ATOM	2416	0	ASN A 3		35.647	26.565	26.534	1.00 7.92	A
ATOM	2417	N	ALA A 3		36.242	24.523	25.806	1.00 8.29	A
ATOM	2418	ÇA	ALA A 3		36.194	23.863	27.117	1.00 8.92	A
MOTA	2419	CB	ALA A 3		37.188	24.526	28.069	1.00 10.50	A
ATOM	2420	С	ALA A 3	38	34.825	23.786	27.785	1.00 8.55	A
ATOM	2421	Ō	ALA A 3		34.732	23.671	29.000	1.00 10.41	Ä
ATOM	2422	Ň	PHE A 3		33.765	23.844	27.002	1.00 7.84	Ä
ATOM	2423	CA	PHE A 3		32.410	23.781	27.553	1.00 8.93	
ATOM	2424	CB	PHE A 3						A
					31.624	25.034	27.120	1.00 7.76	A
ATOM	2425	CG	PHE A 3		32.258	26.345	27.576	1.00 10.23	A
ATOM	2426	CD1	PHE A 3		32.566	26.557	28.923	1.00 11.28	A
ATOM	2427	CD2	PHE A 33	39	32.497	27.369	26.664	1.00 9.75	A

MOTA	2428	CE1	PHE A 339	33.108	27.795	29.360	1.00 11.58	A
MOTA	2429	CE2		33.033	28.613	27.077	1.00 8.17	A
ATOM	2430	CZ	PHE A 339	33.339	28.820	28.437	1.00 8.56	A
ATOM	2431	С	PHE A 339	31.647	22.514	27.151	1.00 9.93	A
ATOM	2432	0	PHE A 339	32.084	21.742	26.279	1.00 9.23	A
MOTA	2433	N	VAL A 340	30.508	22.304	27.797	1.00 8.19	A
ATOM	2434	CA	VAL A 340	29.669	21.139	27.531	1.00 10.26	A
ATOM	2435	CB	VAL A 340	29.169	20.468	28.851	1.00 11.72	A
MOTA	2436	CG1		28.219	19.269	28.538	1.00 8.46	A
MOTA	2437	CG2	VAL A 340	30.346	19.998	29.679	1.00 8.91	A
MOTA	2438	С	VAL A 340	28.439	21.577	26.742	1.00 6.33	A
MOTA	2439	0	VAL A 340	27.675	22.433	27.186	1.00 6.81	Α
MOTA	2440	N_	PRO A 341	28.255	21.021	25.547	1.00 6.85	A
ATOM	2441	CD	PRO A 341	29.193	20.162	24.797	1.00 10.26	A
MOTA	2442	CA	PRO A 341	27.082	21.373	24.736	1.00 9.67	Α
ATOM ATOM	2443	CB	PRO A 341	27.275	20.537	23.468	1.00 11.39	Α
ATOM	2444 2445	CG	PRO A 341 PRO A 341	28.752	20.386	23.363	1.00 14.97	A
ATOM	2446	C	PRO A 341	25.807	20.931	25.497	1.00 10.96	A
ATOM	2447	Ň	LEU A 341	25.851 24.673	20.024	26.342	1.00 10.96	A
ATOM	2448	CA	LEU A 342	23.435	21.558	25.211	1.00 8.13	Ā
ATOM	2449	CB	LEU A 342	22.326	21.157 22.194	25.870 25.646	1.00 10.08	A
ATOM	2450	ČĞ	LEU A 342	22.558	23.605	26.207	1.00 12.81 1.00 16.13	A
ATOM	2451	CD1		21.280	24.428	26.007	1.00 10.13	A N
ATOM	2452	CD2		22.908	23.542	27.715	1.00 10.04	A A
ATOM	2453	С	LEU A 342	22.981	19.821	25.288	1.00 11.00	Ä
MOTA	2454	0	LEU A 342	23.142	19.565	24.072	1.00 10.04	Ä
MOTA	2455	N	PRO A 343	22.437	18.937	26.147	1.00 10.12	A
ATOM	2456	CD	PRO A 343	22.407	19.074	27.618	1.00 8.23	A
ATOM	2457	CA	PRO A 343	21.947	17.622	25.721	1.00 11.60	A
ATOM	2458	CB	PRO A 343	21.407	17.006	27.021	1.00 11.29	A
ATOM	2459	CG	PRO A 343	22.287	17.643	28.083	1.00 12.10	A
ATOM	2460	Č	PRO A 343	20.850	17.839	24.688	1.00 11.38	A
ATOM ATOM	2461 2462	O N	PRO A 343	20.229	18.896	24.648	1.00 10.75	A
ATOM	2463	CA	SER A 344 SER A 344	20.590	16.836	23.861	1.00 9.55	Ā
ATOM	2464	CB	SER A 344	19.592 19.547	16.995 15.741	22.801	1.00 8.34	A
ATOM	2465	og	SER A 344	19.245	14.625	21.940 22.760	1.00 15.39 1.00 23.25	A
ATOM	2466	Č	SER A 344	18.185	17.315	23.281	1.00 23.23	A A
ATOM	2467	ō	SER A 344	17.474	18.051	22.615	1.00 11.06	Ä
ATOM	2468	N	ASN A 345	17.751	16.744	24.410	1.00 11.97	Ä
ATOM	2469	CA	ASN A 345	16.403	17.061	24.874	1.00 13.51	A
ATOM	2470	CB	ASN A 345	15.962	16.128	26.015	1.00 11.25	A
ATOM	2471	CG	ASN A 345	16.896	16.145	27.206	1.00 19.63	А
ATOM	2472	OD1	ASN A 345	18.105	16.399	27.083	1.00 15.65	A
ATOM	2473	ND2		16.343	15.822	28.379	1.00 15.03	A
ATOM ATOM	2474 2475	C	ASN A 345 ASN A 345	16.296 15.236	18.532	25.277	1.00 12.03	Ā
ATOM	2476	Ŋ	TRP A 346	17.397	19.131 19.115	25.167 25.739	1.00 11.72 1.00 10.97	A
ATOM	2477	CA	TRP A 346	17.397	20.533	26.097	1.00 10.97 1.00 9.55	A A
ATOM	2478	CB	TRP A 346	18.663	20.890	26.881	1.00 8.50	A
ATOM	2479	ČĠ	TRP A 346	18.475	20.695	28.372	1.00 9.10	Ä
ATOM	2480	CD2	TRP A 346	17.927	21.660	29.285	1.00 10.08	A
MOTA	2481	CE2	TRP A 346	17.831	21.036	30.549	1.00 12.11	A
MOTA	2482	CE3	TRP A 346	17.502	22.994	29.149	1.00 9.60	A
ATOM	2483	CD1	TRP A 346	18.694	19.553	29.099	1.00 9.06	А
ATOM	2484	NEI	TRP A 346	18.304	19.752	30.411	1.00 9.93	A
ATOM	2485	CZ2	TRP A 346	17.323	21.705	31.682	1.00 9.30	A
ATOM ATOM	2486	CZ3 CH2	TRP A 346	17.004	23.662	30.261	1.00 10.14	Ā
ATOM	2487 2488	Cn2	TRP A 346 TRP A 346	16.917 17.298	23.012	31.522	1.00 12.99	A
ATOM	2489	ŏ	TRP A 346	16.509	21.390 22.333	24.824 24.769	1.00 10.69	A
ATOM	2490	Ň	LYS A 347	18.087	21.074	23.804	1.00 13.16 1.00 9.34	A
ATOM	2491	CA	LYS A 347	17.984	21.852	22.557	1.00 9.34	A A
ATOM	2492	CB	LYS A 347	18.902	21.287	21.466	1.00 12.86	Â
ATOM	2493	ČĞ	LYS A 347	20.416	21.357	21.748	1.00 12.88	À
ATOM	2494	CD	LYS A 347	21.221	21.071	20.440	1.00 14.73	Ä
ATOM	2495	CE	LYS A 347	22.733	21.317	20.590	1.00 14.12	A
MOTA	2496	NZ	LYS A 347	23.467	20.312	21.462	1.00 10.37	A
ATOM	2497	C	LYS A 347	16.549	21.789	22.030	1.00 10.83	A
ATOM	2498	0	LYS A 347	15.956	22.814	21.631	1.00 8.78	A
ATOM	2499	N	ALA A 348	15.987	20.583	21.997	1.00 9.70	A
ATOM	2500 2501	CA CB	ALA A 348 ALA A 348	14.627	20.418	21.472	1.00 9.41	A
ATOM ATOM	2501 2502	CB	ALA A 348	14.238 13.589	18.928 21.224	21.448 22.251	1.00 12.04 1.00 10.82	A N
ATOM	2502	Ö	ALA A 348	12.678	21.224	21.657	1.00 10.82 1.00 9.58	A A
		-		_2.0.0	~~.000	057	2.00 7.30	_

MOTA	2504	N	ALA A	349	13.735	21.261	23.569	1 00 0 30	_
ATOM	2505	CA	ALA A		12.791	22.018	24.392	1.00 9.39 1.00 8.51	A
MOTA	2506	CB	ALA A		13.045	21.750	25.891	1.00 8.51	A A
ATOM	2507	С	ALA A	349	12.909	23.518	24.095	1.00 10.22	A
ATOM	2508	0	ALA A	349	11.888	24.224	24.012	1.00 8.91	Â
ATOM	2509	N	VAL A		14.140	24.002	23.930	1.00 12.16	· A
MOTA	2510	CA	VAL A		14.347	25.423	23.649	1.00 8.94	Ä
ATOM ATOM	2511	CB	VAL A		15.863	25.794	23.629	1.00 8.30	A
ATOM	2512 2513	CG1 CG2			16.075	27.221	23.071	1.00 8.00	A
ATOM	2514	C	VAL A		16.439	25.729	25.075	1.00 8.81	A
ATOM	2515	ŏ	VAL A		13.709 13.046	25.763	22.305	1.00 10.89	A
ATOM	2516	N	ARG A		13.890	26.787 24.895	22.177 21.313	1.00 11.46 1.00 10.91	A
ATOM	2517	CA	ARG A		13.289	25.144	20.002	1.00 10.91 1.00 11.54	A A
ATOM	2518	CB	ARG A		13.765	24.106	18.988	1.00 10.07	Ä
ATOM	2519	CG	ARG A		15.237	24.167	18.647	1.00 10.05	A
ATOM ATOM	2520 2521	CD	ARG A		15.527	23.433	17.312	1.00 14.16	A
ATOM	2522	NE CZ	ARG A ARG A		14.971	22.067	17.282	1.00 17.52	A
ATOM	2523	NH1			15.577 14.993	20.991 19.802	17.780	1.00 14.15	Ā
ATOM	2524	NH2			16.775	21.097	17.708 18.338	1.00 14.19 1.00 15.54	A
MOTA	2525	С	ARG A		11.750	25.097	20.069	1.00 13.34	A A
ATOM	2526	0	ARG A		11.061	25.925	19.477	1.00 10.64	Ä
ATOM	2527	N	ALA A		11.221	24.112	20.786	1.00 10.94	A
ATOM ATOM	2528	CA	ALA A		9.772	23.942	20.890	1.00 13.45	A
ATOM	2529 2530	CB C	ALA A ALA A		9.447	22.656	21.636	1.00 14.54	Α
ATOM	2531	ŏ	ALA A		9.028 7.875	25.112 25.385	21.527	1.00 14.05	A
ATOM	2532	Ň	SER A		9.669	25.802	21.193 22.454	1.00 9.92 1.00 9.51	A
ATOM	2533	CA	SER A		9.024	26.932	23.094	1.00 10.39	A A
MOTA	2534	CB	SER A		9.503	27.08B	24.548	1.00 11.56	Ä
MOTA MOTA	2535 2536	og	SER A		8.802	26.220	25.436	1.00 14.83	A
MOTA	2537	C	SER A SER A		9.308 8.403	28.245	22.386	1.00 12.07	A
ATOM	2538	Ŋ	TYR A		10.568	29.033 28.459	22.178 22.015	1.00 12.33 1.00 10.56	A
MOTA	2539	CA	TYR A		10.955	29.733	21.455	1.00 10.56 1.00 8.65	A A
ATOM	2540	CB	TYR A		12.240	30.188	22.159	1.00 11.42	A
ATOM	2541	CG	TYR A		12.077	30.164	23.670	1.00 11.26	A
ATOM ATOM	2542 2543	CD1	TYR A		11.168	31.007	24.296	1.00 11.16	Α
ATOM	2544	CE1 CD2	TYR A		10.962 12.795	30.955	25.673	1.00 13.86	Ā
ATOM	2545	CE2	TYR A		12.608	29.265 29.204	24.455 25.846	1.00 12.94 1.00 13.83	A
MOTA	2546	CZ	TYR A		11.692	30.048	26.437	1.00 15.83	A A
ATOM	2547	ОН	TYR A		11.496	29.985	27.784	1.00 31.84	Ä
ATOM	2548	C	TYR A		11.069	29.882	19.951	1.00 11.12	A
ATOM ATOM	2549 2550	O N	TYR A LEU A		11.137	31.011	19.456	1.00 11.00	A
ATOM	2551	CA	LEU A		11.097 11.156	28.778 28.896	19.218 17.757	1.00 9.87 1.00 11.35	A
MOTA	2552	CB	LEU A		12.292	28.069	17.185	1.00 11.35	A A
MOTA	2553	CG	LEU A	355	13.697	28.633	17.424	1.00 18.77	Ä
ATOM	2554	CD1	LEU A		14.731	27.617	16.930	1.00 13.44	A
ATOM ATOM	2555 2556	CD2	LEU A		13.856	29.963	16.666	1.00 19.42	A
ATOM	2557	C O	LEU A		9.848 9.337	28.484	17.086	1.00 12.49	Ā
ATOM	2558	Ň	THR A		9.300	29.208 27.331	16.231 17.458	1.00 13.91 1.00 13.88	A
ATOM	2559	CA	THR A		8.036	26.866	16.849	1.00 15.88	A A
MOTA	2560	CB	THR A	356	7.414	25.759	17.704	1.00 19.06	Ä
ATOM	2561	OG1	THR A		8.352	24.678	17.794	1.00 22.02	A
ATOM ATOM	2562 2563	CG2	THR A		6.108	25.265	17.077	1.00 20.44	A
ATOM	2564	C	THR A		7.058 6.609	28.040	16.684	1.00 15.88	Ā
MOTA	2565	N	ALA A		6.720	28.642 28.362	17.658 15.441	1.00 14.53 1.00 16.53	A
ATOM	2566	CA	ALA A		5.892	29.536	15.175	1.00 15.13	A A
MOTA	2567	CB	ALA A		5.654	29.669	13.662	1.00 17.87	Ä
ATOM	2568	Č	ALA A		4.569	29.630	15.918	1.00 18.27	A
MOTA MOTA	2569 2570	O	ALA A		4.141	30.714	16.295	1.00 19.17	A
ATOM	2570 2571	N CA	SER A SER A		3.930 2.643	28.492 28.444	16.127	1.00 18.84	A
MOTA	2572	CB	SER A		1.953	28.444	16.800 16.459	1.00 22.62 1.00 18.79	A
MOTA	2573	ÕĞ	SER A		2.853	26.049	16.654	1.00 18.79	A A
MOTA	2574	C	SER A	358	2.716	28.607	18.318	1.00 22.54	Ä
MOTA	2575	0	SER A		1.719	28.918	18.949	1.00 19.82	A
MOTA MOTA	2576 2577	N Ca	ASN A		3.886	28.410	18.916	1.00 20.48	A
ATOM	2578		ASN A ASN A		3.950 5.249	28.550 27.956	20.358	1.00 16.65	A
ATOM	2579		ASN A		5.180	27.718	20.909 22.387	1.00 12.27 1.00 11.80	A A
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ATOM	2580	OD1	3011 3 30					
			ASN A 35		28.652	23.170	1.00 16.11	A
MOTA	2581	ND2			26.451	22.793	1.00 14.58	A
ATOM	2582	С	ASN A 35	3.844	30.019	20.745	1.00 16.93	A
MOTA	2583	0	ASN A 35	9 4.550	30.861	20.194	1.00 15.08	A
ATOM	2584	N	ALA A 36		30.306	21.712	1.00 15.71	Ä
ATOM	2585	CA	ALA A 36					
ATOM	2586				31.664	22.208	1.00 18.67	A
		CB	ALA A 36		31.651	23.320	1.00 22.67	A
MOTA	2587	Č	ALA A 36		32.309	22.744	1.00 18.59	A
MOTA	2588	. 0	ALA A 36	4.138	33.532	22.825	1.00 16.11	A
ATOM	2589	N	LEU A 36	L 5.010	31.488	23.144	1.00 14.62	A
ATOM	2590	CA	LEU A 36		32.021	23.653	1.00 11.27	A
ATOM	2591	CB	LEU A 36		31.060	24.685	1.00 15.51	
ATOM	2592	ČĞ	LEU A 36		30.788			A
ATOM	2593	CD1				25.971		A
ATOM					29.586	26.688	1.00 15.50	A
	2594	CD2	LEU A 36		32.030	26.849	1.00 14.07	A
ATOM	2595	Č	LEU A 36		32.219	22.545	1.00 12.87	A
ATOM	2596	0	LEU A 36		32.716	22.818	1.00 12.41	A
MOTA	2597	N	SER A 36	7.036	31.821	21.314	1.00 9.97	A
ATOM	2598	CA	SER A 36	8.044	31.936	20.257	1.00 10.76	Α
MOTA	2599	CB	SER A 36	7.627	31.145	19.011	1.00 15.72	A
MOTA	2600	OG	SER A 36		31.707	18.416	1.00 18.79	Ä
MOTA	2601	С	SER A 36		33.338	19.822	1.00 12.29	Ä
ATOM	2602	õ	SER A 36		34.258	19.742	1.00 12.25	
MOTA	2603	Ň	ILE A 36		33.457	19.512		A
ATOM	2604	ĈA	ILE A 36					A
ATOM					34.698	19.072	1.00 14.99	A
	2605	CB	ILE A 36		34.461	18.777	1.00 13.05	A
ATOM	2606	CG2	ILE A 36		35.713	18.198	1.00 12.46	A
MOTA	2607	CG1	ILE A 36		34.071	20.064	1.00 15.60	A
MOTA	2608	CD1	ILE A 36		33.442	19.815	1.00 11.48	A
ATOM	2609	С	ILE A 36	9.639	35.206	17.807	1.00 14.29	A
MOTA	2610	0	ILE A 36	9.509	34.481	16.830	1.00 12.01	A
ATOM	2611	N	GLY A 36	9.176	36.451	17.848	1.00 15.53	A
ATOM	2612	CA	GLY A 36		37.034	16.717	1.00 14.88	A
ATOM	2613	Ċ	GLY A 36		36.567	16.514	1.00 19.34	Ä
ATOM	2614	ŏ	GLY A 36		36.872	15.487	1.00 19.36	Ä
ATOM	2615	N	ASP A 36		35.842	17.474	1.00 15.42	
ATOM	2616	CA	ASP A 36		35.360			A
ATOM	2617	CB				17.323	1.00 16.08	A
			ASP A 36		34.691	18.613	1.00 17.24	Ā
ATOM	2618	CG	ASP A 36		34.201	18.516	1.00 22.13	A
ATOM	2619	OD1	ASP A 36		33.003	18.238	1.00 24.97	A
ATOM	2620	OD2	ASP A 36		35.025	18.698	1.00 22.46	A
MOTA	2621	С	ASP A 36	4.100	36.490	16.954	1.00 20.12	A
MOTA	2622	0	ASP A 36	3.979	37.482	17.668	1.00 17.92	A·
MOTA	2623	N	SER A 36	3.379	36.317	15.848	1.00 21.25	A
MOTA	2624	CA	SER A 36		37.319	15.360	1.00 19.32	A
ATOM	2625	CB	SER A 36		36.787	14.108	1.00 21.13	A
ATOM	2626	ŌĞ	SER A 36		36.400	13.125	1.00 29.92	Ä
ATOM	2627	č	SER A 36		37.814	16.342	1.00 25.32	Ä
ATOM	2628	ŏ	SER A 36		39.010	16.461		
ATOM	2629	Ŋ	ALA A 36					A
					36.920	17.024	1.00 18.40	Ä
ATOM	2630	CA	ALA A 36		37.363	17.965	1.00 22.33	A
ATOM	2631	CB	ALA A 36		36.175	18.431	1.00 19.13	A
ATOM	2632	Č	ALA A 36		38.093	19.187	1.00 25.24	A
ATOM	2633	0	ALA A 36		39.066	19.682	1.00 26.45	A
MOTA	2634	N	VAL A 36		37.612	19.692	1.00 24.39	A
MOTA	2635	CA	VAL A 36		38.229	20.864	1.00 21.43	A
MOTA	2636	CB	VAL A 36	2.729	37.182	21.657	1.00 23.84	Α
ATOM	2637	CG1	VAL A 36	3.447	37.838	22.850	1.00 19.42	A
ATOM	2638	CG2	VAL A 36		36.094	22.148	1.00 25.28	A
ATOM	2639	С	VAL A 36		39.447	20.558	1.00 19.50	A
ATOM	2640	ō	VAL A 36		40.440	21.277	1.00 22.77	A
ATOM	2641	Ň	CYS A 36		39.396	19.491	1.00 17.47	Ä
ATOM	2642	CA	CYS A 36		40.505			
						19.195	1.00 20.32	A
ATOM	2643	Č	CYS A 36		41.648	18.322	1.00 23.64	A
ATOM	2644	0	CYS A 36		42.639	18.120	1.00 26.98	Ā
ATOM	2645	CB	CYS A 36		39.977	18.581	1.00 22.42	A
ATOM	2646	SG	CYS A 36		38.961	19.671	1.00 19.53	A
MOTA	2647	N	GLY A 370		41.521	17.812	1.00 25.38	A
ATOM	2648	CA.	GLY A 370		42.575	16.966	1.00 27.80	A
ATOM	2649	С	GLY A 370	2.190	43.938	17.627	1.00 21.46	Α
ATOM	2650	Ō	GLY A 376		44.112	18.705	1.00 25.76	A
ATOM	2651	Ň	GLY A 37		44.885	16.988	1.00 20.44	Ä
ATOM	2652	CA	GLY A 37		46.237	17.516	1.00 23.12	Ä
ATOM	2653	Č.	GLY A 37		46.463	18.695	1.00 26.63	Ä
ATOM	2654	ŏ	GLY A 37		47.561	19.263	1.00 23.97	Â
ATOM	2655	N	LYS A 372		45.443	19.057	1.00 23.24	A
A1011	2033	7.4	510 K 3/	4.009	47.443	19.057	1.00 23.24	A

ATOM	2656	CA	T VO 3 200					
			LYS A 372	5.612	45.537	20.197	1.00 21.66	A
MOTA	2657	CB	LYS A 372	5.141	44.605	21.296	1.00 19.20	A
ATOM	2658	CG	LYS A 372	3.715	44.856	21.675	1.00 25.31	A
ATOM	2659	CD	LYS A 372					
				3.278	43.936	22.769	1.00 24.34	A
ATOM	2660	CE	LYS A 372	1.884	44.315	23.208	1.00 29.63	A
ATOM	2661	NZ	LYS A 372	1.426	43.423	24.285	1.00 25.95	A
ATOM	2662	C	LYS A 372					
				7.037	45.167	19.855	1.00 18.74	A
ATOM	2663	0	LYS A 372	7.337	44.799	18.721	1.00 17.43	Α
ATOM	2664	N	GLY A 373	7.917	45.247	20.852	1.00 15.44	A
ATOM	2665	CA	GLY A 373	9.297	44.876			
ATOM						20.616	1.00 12.87	A
	2666	Č	GLY A 373	10.366	45.876	21.015	1.00 17.42	A
MOTA	2667	0	GLY A 373	10.168	47.106	20.965	1.00 13.70	A
ATOM	2668	N	ARG A 374	11.517	45.342	21.419	1.00 14.49	A
ATOM	2669	CA	ARG A 374	12.639				
					46.187	21.792	1.00 13.29	A
ATOM	2670	CB	ARG A 374	13.786	45.339	22.333	1.00 15.72	A
ATOM	2671	CG	ARG A 374	13.456	44.710	23.692	1.00 18.10	A
ATOM	2672	CD	ARG A 374	14.668	44.080	24.332	1.00 20.11	A
ATOM	2673	NE	ARG A 374					
				15.729	45.034	24.665	1.00 13.47	, A
ATOM	2674	CZ	ARG A 374	16.143	45.296	25.899	1.00 13.50	A
ATOM	2675	NH1	ARG A 374	15.564	44.694	26.928	1.00 11.14	A
ATOM	2676	NH2	ARG A 374	17.206	46.082	26.100	1.00 9.65	A
ATOM	2677	C						
			ARG A 374	13.097	46.989	20.563	1.00 14.09	A
ATOM	2678	0	ARG A 374	13.008	46.517	19.411	1.00 13.90	A
ATOM	2679	N	PRO A 375	13.575	48.225	20.797	1.00 13.52	A
ATOM	2680	CD	PRO A 375	13.680	48.834	22.133	1.00 12.37	A
ATOM	2681	CA						
			PRO A 375	14.051	49.137	19.753	1.00 15.51	A
ATOM	2682	CB	PRO A 375	14.304	50.445	20.516	1.00 18.56	A
ATOM	2683	CG	PRO A 375	14.669	49.958	21.903	1.00 16.56	A
ATOM	2684	С	PRO A 375	15.282	48.622	19.017	1.00 16.94	
ATOM	2685	ŏ	PRO A 375					A
				16.130	47.953	19.605	1.00 16.29	А
ATOM	2686	N	GLU A 376	15.384	48.956	17.733	1.00 14.83	A
ATOM	2687	CA	GLU A 376	16.501	48.480	16.928	1.00 14.54	A
ATOM	2688	CB	GLU A 376	16.191	48.638	15.429	1.00 20.94	A
ATOM	2689	CG						
			GLU A 376	15.989	50.054	14.930	1.00 25.93	A
ATOM	2690	CD	GLU A 376	15.840	50.093	13.408	1.00 28.12	A
ATOM	2691	OE1	GLU A 376	16.852	50.265	12.693	1.00 27.73	A
ATOM	2692	OE2	GLU A 376	14.706	49.921	12.926		
ATOM								Ā
	2693	C	GLU A 376	17.818	49.144	17.258	1.00 15.46	A
ATOM	2694	0	GLU A 376	17.779	50.308	17.715	1.00 20.34	A
ATOM	2695	OXT	GLU A 376	18.870	48.501	17.040	1.00 17.16	A
ATOM	2696	OH2	WAT S1500	35.620	33.372	34.950	1.00 7.74	s
ATOM	2697							2
		OH2		26.719	26.585	54.115	1.00 13.35	s
ATOM	2698	OH2	WAT S1502	32.910	38.720	42.612	1.00 11.02	s
ATOM	2699	OH2	WAT S1503	25.842	40.990	19.393	1.00 10.30	s
ATOM	2700	OH2	WAT S1504	47.855	24.508	32.439	1.00 11.64	Š
ATOM	2701	OH2	WAT S1505	37.575				2
					38.877	30.460	1.00 13.25	S
ATOM	2702	OH2	WAT S1506	43.970	19.166	36.360	1.00 11.89	S
ATOM	2703	OH2	WAT S1507	51.431	26.280	38.870	1.00 11.08	s
ATOM	2704	OH2	WAT S1508	21.180	34.238	33.496	1.00 10.94	S
ATOM	2705	OH2	WAT S1509	34.016	23.145	55.150		
							1.00 7.21	· S
ATOM	2706	OH2	WAT S1510	34.137	35.767	50.996	1.00 14.32	, S
ATOM	2707	OH2	WAT \$1511	29.833	31.064	61.815	1.00 12.62	S
ATOM	2708	OH2	WAT S1512	36.421	34.348	51.750	1.00 8.81	s
ATOM	2709	OH2	WAT S1513	24.593	22.841	22.601	1.00 14.49	š
MOTA	2710	OH2	WAT S1514	33.875	20.919	53.336	1.00 15.73	s
ATOM	2711		WAT \$1515	55.590	18.894	44.228	1.00 20.22	S
ATOM	2712	OH2	WAT \$1516	25.163	24.507	19.298	1.00 7.32	s
ATOM	2713		WAT S1517	29.287	27.565	53.584	1.00 10.43	s
ATOM	2714		WAT S1518	27.630	35.157	54.573	1.00 11.84	s
								5
ATOM	2715		WAT S1519	34.308	40.814	45.314	1.00 9.91	S
ATOM	2716		WAT S1520	24.097	26.340	47.444	1.00 12.35	S
ATOM	2717	OH2	WAT S1521	26.289	17.353	26.191	1.00 14.15	S
ATOM	2718		WAT S1522	31.025	26.248	57.309	1.00 9.97	s s
								3
ATOM	2719		WAT S1523	16.012	33.323	36.822	1.00 10.61	S
ATOM	2720		WAT S1524	35.079	31.981	26.882	1.00 7.27	ននិងនិងនិង
ATOM	2721	OH2	WAT S1525	48.948	16.302	35.666	1.00 22.32	s
ATOM	2722		WAT S1526	23.036	32.247	50.228	1.00 12.80	č
								ž
ATOM	2723		WAT S1527	41.445	42.204	48.819	1.00 16.71	S
ATOM	2724	OH2	WAT S1528	30.777	34.835	16.827	1.00 12.96	s
ATOM	2725	OH2	WAT S1529	9.482	33.895	27.983	1.00 10.22	S
ATOM	2726		WAT S1530	10.107	31.646	29.601	1.00 12.12	Š
				10.10/				2
ATOM	2727		WAT S1531	37.836	31.446	58.127	1.00 18.63	s
ATOM	2728		WAT S1532	23.419	29.528	35.937	1.00 10.10	S
MOTA	2729	OH2	WAT S1533	36.234	16.727	51.505	1.00 9.28	S
ATOM	2730	OH2	WAT S1534	5.728	38.503	24.985	1.00 13.33	š
ATOM	2731	OHZ	WAT S1535	29.914	14.295	35.432	1.00 16.41	S

OH2 WAT S1536 OH2 WAT S1537 2732 2733 2734 2735 2736 ATOM 31.310 1.00 9.93 38.281 18.695 MOTA 44.863 16.606 36.022 1.00 15.09 ATOM OH2 WAT S1538 40.186 22.869 38.700 1.00 9.90 ATOM 37.549 OH2 WAT S1539 20.501 28.090 1.00 MOTA OH2 WAT S1540 12.913 31.829 29.436 1.00 2737 MOTA OH2 TAW S1541 30.589 15.671 37.530 1.00 MOTA 2738 OH2 WAT S1542 23.885 35.406 43.402 1.00 18.37 ATOM 2739 OH2 WAT S1543 8.663 34.010 25.289 1.00 13.37 33.757 57.944 7.715 41.885 13.484 **ATOM** 2740 OH2 WAT S1544 46.444 1.00 12.24 27.923 17.540 MOTA 2741 OH2 WAT S1545 19.477 1.00 11.68 ATOM 2742 WAT S1546 OH2 33.345 19.22 1.00 51.552 27.270 ATOM 2743 OH2 WAT S1547 13.602 1.00 25.84 S S1548 MOTA 2744 OH2 WAT 26.074 40.675 1.00 10.51 S 27.760 37.046 37.573 43.771 S1549 S1550 20.816 2745 **ATOM** OH2 WAT 1.00 13.46 S 27.914 MOTA 2746 OH2 TAW 14.34 1.00 S WAT S1550 WAT S1551 WAT S1552 WAT S1553 WAT S1554 MOTA 2747 OH2 33.819 20.741 35.565 23.07 17.08 1.00 40.930 4.472 26.302 2748 ATOM OH2 14.067 1.00 S ATOM 2749 32.567 28.375 OH2 29.061 1.00 18.41 S 32.912 ATOM 2750 OH2 1.00 10.00 ATOM \$1555 2751 OH2 WAT 14.165 29.555 16.934 45.737 13.06 1.00 S 2752 S1556 ATOM OH2 WAT 43.029 36.030 7.32 1.00 S 2753 2754 WAT \$1557 36.451 31.931 23.622 37.298 49.603 37.001 MOTA OH2 34.819 1.00 11.33 WAT S1558 WAT S1559 OH₂ ATOM 17.255 1.00 39.16 s 2755 ATOM OH2 26.926 1.00 11.87 WAT S1560 WAT S1561 WAT S1562 2756 ATOM OH2 31.327 13.311 33.059 1.00 12.47 s 2757 44.899 44.879 36.741 ATOM OH2 41.787 1.00 23.25 2758 35.365 50.011 ATOM OH₂ 50.334 1.00 9.60 WAT S1563 WAT S1564 WAT S1565 WAT S1566 WAT S1566 2759 MOTA OH2 20.827 18.100 1.00 15.06 2760 MOTA 24.374 38.304 OH2 31.041 1.00 12.38 2761 2762 42.003 35.751 26.114 40.722 ATOM OH2 11.411 1.00 14.55 ATOM OH2 21.341 1.00 12.16 2763 2764 2765 2766 MOTA 10.175 47.181 OH2 31.393 39.888 1.00 37.76 WAT S1568 WAT S1569 WAT S1570 33.704 ATOM OH2 26.945 1.00 12.30 36.919 15.706 MOTA OH2 42.028 43.488 1.00 25.46 24.724 MOTA OH2 31.053 1.00 12.46 2767 2768 MOTA OH2 WAT S1571 10.314 39.156 33.480 1.00 10.32 MOTA WAT S1572 OH2 51.433 20.485 50.130 1.00 15.09 2769 2770 2771 2772 2773 2774 MOTA 30.656 53.758 WAT S1573 1.00 OH2 43.925 51.790 17.28 MOTA OH2 WAT S1574 23.091 28.375 1.00 12.50 ATOM OH2 WAT S1575 34.977 41.183 53.019 15.31 1.00 MOTA OH2 WAT S1576 29.766 26.781 12.309 1.00 18.82 MOTA OH2 **WAT S1577** 9.190 36.561 30.593 1.00 11.25 MOTA OH2 TAW S1578 36.599 15.728 48.666 1.00 21.18 MOTA 2775 OH2 WAT S1579 37.724 34.865 54.143 1.00 11.62 21.457 MOTA 2776 OH2 WAT S1580 35.713 12.303 1.00 13.24 MOTA 2777 OH2 WAT S1581 27.734 31.073 59.797 1.00 14.78 s ATOM 2778 OH2 WAT S1582 51.536 35.554 40.163 1.00 14.52 s 53.057 ATOM 2779 OH2 WAT S1583 29.933 42.651 1.00 14.55 ATOM 2780 OH2 WAT S1584 9.469 20.704 23.677 25.125 1.00 12.14 S 29.372 22.975 2781 OH2 WAT S1585 11.334 1.00 17.80 ATOM S 56.481 9.572 38.435 1.00 2782 WAT ATOM OH2 S1586 29.16 S 40.421 42.224 37.848 2783 WAT S1587 ATOM OH2 14.99 S 20.542 1.00 MOTA 2784 OH2 WAT S1588 40.862 13.90 S 39.841 28.636 15.10 MOTA 2785 OH2 WAT S1589 1.00 9.567 6.391 41.492 22.505 27.720 37.216 30.199 48.835 20.894 28.556 1.00 **ATOM** 2786 OH2 WAT S1590 19.52 S 55.469 52.952 1.00 ATOM 2787 OH2 WAT S1591 16.40 S 1.00 **ATOM** 2788 OH2 WAT S1592 24.23 15.40 S 2789 WAT 20.204 ATOM OH2 S1593 46.441 1.00 S 41.499 27.159 1.00 MOTA 2790 OH2 WAT S1594 30.864 19.68 S WAT S1595 **ATOM** 2791 OH2 15.034 11.19 1.00 S 2792 30.964 WAT 25.139 35.730 **ATOM** OH2 S1596 53.858 1.00 21.47 2793 WAT S1597 20.698 ATOM OH2 18.767 15.15 17.67 1.00 S WAT S1598 S1599 44.994 28.802 23.797 26.514 MOTA 2794 OH2 20.666 1.00 MOTA 2795 58.069 17.28 OH2 1.00 S WAT WAT 16.767 30.159 47.104 33.756 22.319 60.797 2796 OH2 S1600 MOTA 1.00 11.98 S 2797 MOTA OH2 S1601 1.00 9.19 27.997 2798 WAT S1602 36.005 MOTA OH2 48.106 1.00 14.93 21.552 18.008 2799 WAT 40.650 24.407 MOTA OH2 S1603 1.00 17.12 22.968 **ATOM** 2800 OH2 WAT S1604 17.449 1.00 17.85 **ATOM** 2801 OH2 WAT S1605 16.621 15.788 18.605 1.00 25.68 1.00 14.53 **ATOM** 2802 OH2 WAT S1606 7.206 32.992 16.005 57.149 MOTA 2803 OH2 WAT S1607 24.564 47.629 1.00 18.35 **ATOM** 2804 OH2 WAT S1608 24.205 26.840 10.350 1.00 23.21 2805 WAT S1609 33.745 22.604 **ATOM** OH2 31.364 1.00 14.24 WAT \$1610 21.687 28.608 49.750 MOTA 2806 OH₂ 1.00 41.13 MOTA 2807 OH2 WAT S1611 25.572 18.289 18.085 1.00 18.47

MOTA	2808	OH2	WAT	S1612	29.378	22 040	15 270	1 00 10 53	_
ATOM	2809	OH2				22.049	15.378	1.00 18.53	S
ATOM	2810	OH2			47.580	17.180	46.156	1.00 18.00	s
ATOM	2811	OH2			23.216	43.309	37.644	1.00 13.17	s
ATOM	2812				22.669	24.274	48.564	1.00 24.15	S
		OH2			0.336	31.433	18.582	1.00 27.87	s
ATOM	2813	OHZ	WAT	S1617	45.294	33.053	51.773	1.00 13.88	នទទទ
ATOM	2814			S1618	44.363	26.868	22.624	1.00 23.01	S
ATOM	2815	OH2			24.023	16.291	14.532	1.00 14.28	S
MOTA	2816	OH2			25.803	16.259	28.626	1.00 18.77	S
MOTA	2817			S1621	10.423	51.944	32.078	1.00 36.29	S
MOTA	2818	OH2	WAT	S1622	26.115	58.809	27.014	1.00 15.64	S S S
MOTA	2819	OH2	WAT	S1623	1.344	28.356	22.672	1.00 26.37	s
MOTA	2820	OH2	WAT	S1624	26.639	58.198	21.115	1.00 25.02	Š
MOTA	2821	OH2	WAT	S1625	26.622	32.997	55.284	1.00 16.24	Š
MOTA	2822	OH2			15.027	52.473	26.183	1.00 21.76	ន ន ន ន ន ន
ATOM	2823	OH2		S1627	57.187	25.783	44.900	1.00 20.20	2
ATOM	2824	OH2		S1628	44.922	43.322	47.514	1.00 20.20	2
ATOM	2825	OH2		S1629	32.001	38.779	53.199		3
MOTA	2826	OH2		S1630	30.741	52.390			2
ATOM	2827	OH2		S1631	14.999		22.108	1.00 18.11	5
ATOM	2828	OH2		S1632	44.210	39.258	44.162	1.00 19.15	5
ATOM	2829	OH2		S1633	21.471	20.606	55.552	1.00 17.79	5
ATOM	2830	OH2		S1634		43.377	12.416	1.00 19.05	S
ATOM	2831	OH2		S1635	13.869	15.823	31.777	1.00 25.21	S
ATOM					52.620	30.612	55.173	1.00 30.08	១១១១១១១
	2832	OH2		S1636	26.556	19.486	52.050	1.00 29.07	S
ATOM	2833	OH2		S1637	21.965	25.980	45.841	1.00 19.07	S
MOTA	2834	OH2		S1638	51.617	33.897	42.473	1.00 9.81	S
ATOM	2835	OH2		S1639	11.552	20.655	19.351	1.00 16.68	S
ATOM	2836	OH2		S1640	30.899	45.201	19.222	1.00 26.19	១១១១១១១១
ATOM	2837	OH2		S1641	31.709	48.342	31.000	1.00 18.10	S
ATOM	2838	OH2		S1642	23.676	25.327	22.818	1.00 14.28	S
ATOM	2839	OH2	WAT		25.577	17.219	46.479	1.00 20.91	s
ATOM	2840	OH2		S1644	18.005	18.283	19.152	1.00 24.14	S
ATOM	2841	OH2		S1645	52.881	16.705	50.095	1.00 20.16	S
ATOM	2842	OH2	TAW	S1646	5.848	42.562	37.856	1.00 19.01	. S
ATOM	2843	OH2	WAT	S1647	43.582	14.659	34.565	1.00 28.17	S
MOTA	2844	OH2	WAT	S1648	22.374	17.743	20.886	1.00 18.81	s
ATOM	2845	OH2	WAT	S1649	8.712	48.989	27.030	1.00 23.87	ŝ
ATOM	2846	OH2	WAT	S1650	2.521	47.157	34.228	1.00 30.10	Š
ATOM	2847	OH2		S1651	44.220	43.064	40.109	1.00 29.97	Š
ATOM	2848	OH2	WAT		27.919	24.353	12.179	1.00 16.62	, Š
ATOM	2849	OH2		S1653	3.523	42.077	26.249	1.00 22.83	Š
ATOM	2850	OH2	WAT		20.380	44.291	37.672	1.00 17.30	s
ATOM	2851	OH2		S1655	57.034	28.423	45.056	1.00 27.44	Š
ATOM	2852			S1656	49.668	24.467	30.455	1.00 22.73	
ATOM	2853	OH2		S1657	51.259	13.409	45.586	1.00 34.23	SSSS
ATOM	2854	OH2		S1658	9.456	23.136	36.163	1.00 24.71	S
MOTA	2855			S1659	52.331	23.665	57.905	1.00 18.92	2
ATOM	2856	OH2		S1660	43.381	40.535	56.268	1.00 30.03	\$ \$ \$ \$ \$ \$ \$
ATOM	2857	OH2		S1661	13.806	46.776	43.159	1.00 30.03	2
ATOM	2858			S1662	53.981	30.491	48.223		2
ATOM	2859	OH2	WAT		41.765	26.570	28.744		5
ATOM	2860		WAT		40.737	17.318	53.732	1.00 27.76	5
ATOM	2861			S1665	13.225	44.990		1.00 24.67	S
ATOM	2862			S1666			8.674	1.00 28.84	S
MOTA	2863			S1667	49.013	41.254	39.651	1.00 28.00	S
ATOM	2864				44.805	37.426	30.933	1.00 16.56	S
ATOM				S1668	43.625	18.020	54.500	1.00 24.62	s
	2865	OH2		S1669	14.317	25.699	46.118	1.00 34.64	s
ATOM	2866			S1670	3.256	42.913	32.109	1.00 29.06	s
ATOM	2867			S1671	10.555	49.763	20.725	1.00 2B.19	S
ATOM	2868			S1672	10.096	51.223	27.611	1.00 23.49	s
MOTA	2869			S1673	14.363	23.946	36.209	1.00 40.49	S
MOTA	2870			S1674	25.126	59.432	22.831	1.00 22.37	S
ATOM	2871			S1675	36.093	4.004	46.425	1.00 41.05	s
ATOM	2872			S1676	58.346	33.177	43.906	1.00 32.25	S
MOTA	2873			S1677	48.932	35.192	51.801	1.00 26.68	S
ATOM	2874	OH2		S1678	58.902	19.301	43.107	1.00 25.48	S
MOTA	2875	OH2		S1679	44.340	42.085	50.822	1.00 28.00	S
MOTA	2876	OH2		S1680	50.480	38.266	34.016	1.00 31.92	S
ATOM	2877	OH2	WAT	S1681	32.259	20.178	55.706	1.00 22.68	S
MOTA	2878	OH2		S1682	5.907	48.823	21.778	1.00 41.37	S
MOTA	2879	OH2		S1683	50.286	29.738	36.205	1.00 41.24	s
ATOM	2880	OH2		S1684	48.359	24.392	27.682	1.00 21.59	Š
MOTA	2881	OH2		S1685	28.819	16.491	25.944	1.00 22.91	Š
MOTA	2882	OH2		S1686	27.814	39.366	53.598	1.00 22.13	š
MOTA	2883	OH2		S1687	23.282	56.182	29.647	1.00 21.73	š
		_							_

```
OH2 WAT 51688
OH2 WAT 51689
 MOTA
         2884
                                       11.176
                                                51.488
                                                          23.245
                                                                   1.00 39.40
 MOTA
         2885
                                       19.333
                                                13.893
                                                          25.470
                                                                   1.00 16.29
 ATOM
         2886
                OH2
                     WAT S1690
                                       15.528
                                                 35.966
                                                                    1.00
                                                          43.442
                                                                         24.55
 ATOM
         2887
                OH2
                     WAT
                          S1691
                                       28.485
                                                18.098
                                                          54.189
                                                                   1.00 38.82
 ATOM
         2888
                OH2
                     WAT S1692
                                       49.461
                                                 42.346
                                                          42.415
                                                                   1.00 29.71
 ATOM
         2889
                OH2
                     WAT
                          S1693
                                        6.986
                                                          31.491
                                                51.318
                                                                   1.00 38.19
                                                                                       S
 ATOM
         2890
                OH2
                     WAT S1694
                                       45.805
                                                30.330
                                                          30.352
                                                                   1.00 31.74
 ATOM
         2891
                OH2
                     WAT
                          S1695
                                       12.688
                                                17.949
                                                          24.810
                                                                   1.00 24.29
                                                                                       S
 ATOM
         2892
                OH2
                     WAT S1696
                                       10.481
                                                                   1.00 30.36
1.00 22.75
                                                44.192
                                                          41.405
 ATOM
         2893
                OH2
                     WAT
                          S1697
                                       36.497
                                                25.163
                                                          61.042
                                                                                       s
 ATOM
         2894
                OH2
                     WAT S1698
                                                                   1.00 35.83
1.00 25.66
1.00 12.79
1.00 38.68
                                       38.997
                                                 8.895
                                                          40.582
 ATOM
         2895
                OH2
                     WAT
                          S1699
                                       34.429
                                                41.271
                                                          24.603
                                                                                       S
 ATOM
         2896
                OH2
                     WAT S1700
                                        9.264
                                                39.356
                                                          31.031
42.971
                OH2
 ATOM
         2897
                         S1701
                     WAT
                                       10.070
                                                23.977
                                                                                       s
 MOTA
         2898
                         S1702
                OH2
                     WAT
                                                           9.706
                                       18.383
                                                29.372
                                                                   1.00 36.59
1.00 29.13
 MOTA
         2899
                OH2
                     WAT
                         S1703
                                       49.044
                                                14.511
                                                          44.663
                                                                                       S
 MOTA
         2900
                OH2
                    WAT
                         S1704
                                                          39.612
12.779
                                                26.271
                                       24.559
                                                                   1.00
                                                                          9.57
 ATOM
         2901
                OH2
                    WAT
                         S1705
                                       20.114
                                                45.757
                                                                   1.00 24.18
 MOTA
         2902
                OH2
                    WAT
                         S1706
                                       40.248
                                                22.113
                                                          20.074
                                                                   1.00 29.44
1.00 17.46
         2903
 ATOM
                OH2
                    WAT
                         S1707
                                       18.194
                                                41.869
                                                          42.229
 ATOM
         2904
                    WAT
                    WAT S1708
WAT S1709
                OH2
                                       37.847
                                                20.546
                                                         20.498
                                                                   1.00 18.73
 ATOM
         2905
                OH2
                                       16.821
                                                29.280
                                                          41.001
                                                                   1.00 24.06
 MOTA
         2906
                OH2
                    WAT
                         S1710
                                       27.294
                                                         52.815
                                                42.193
                                                                   1.00 19.46
         2907
 MOTA
                    WAT S1711
WAT S1712
                OH2
                                                         51.556
                                       40.821
                                                42.347
                                                                   1.00 22.66
 ATOM
         2908
                OH2
                                       26.156
                                                40.106
                                                         48.095
                                                                   1.00 24.85
ATOM
         2909
                    WAT S1713
                OH2
                                       20.103
                                                24.718
                                                         47.608
                                                                   1.00 30.63
MOTA
         2910
                    WAT S1714
                OH2
                                       24.148
                                                33.741
                                                         56.397
                                                                   1.00 19.34
                                                                                      s
MOTA
         2911
                    WAT S1715
                OH2
                                      18.973
                                                45.993
                                                         36.285
                                                                   1.00 18.68
ATOM
         2912
                                      14.529
                OH2
                    WAT S1716
                                                44.714
                                                         35.623
                                                                   1.00 11.98
                                                                                      s
         2913
ATOM
                OH2
                    WAT S1717
                                      38.781
                                                35.753
                                                         22.003
                                                                   1.00 28.14
         2914
ATOM
                OH2
                    WAT S1718
                                                37.190
                                       9.031
                                                         34.220
                                                                   1.00 30.97
         2915
ATOM
                OH2
                    WAT S1719
                                      35.994
                                                16.311
                                                         25.745
                                                                   1.00 28.93
ATOM
         2916
                OH2
                    WAT
                                      13.544
22.265
                         S1720
                                                49.140
                                                         34.673
                                                                   1.00 19.62
ATOM
         2917
                OH2
                    WAT S1721
                                                37.832
                                                         42.637
                                                                   1.00 21.65
                                      9.246
46.901
27.124
5.808
ATOM
         2918
                OH2
                    WAT
                         S1722
                                                42.739
                                                         13.991
                                                                   1.00 23.76
ATOM
         2919
               OH2 WAT S1723
                                                14.013
                                                         46.528
                                                                   1.00 24.08
ATOM
        2920
               OH2
                    WAT
                         S1724
                                                17.124
                                                         56.373
                                                                   1.00 20.76
ATOM
        2921
               OH2
                    WAT S1725
                                                39.927
                                                         37.880
                                                                   1.00 30.10
MOTA
        2922
               OH2
                    WAT
                         S1726
                                      42.361
                                                20.811
                                                         20.431
                                                                   1.00
                                                                        24.61
ATOM
        2923
               OH2
                    WAT S1727
                                      26.665
                                                17.537
                                                         21.374
                                                                   1.00
                                                                         22.27
MOTA
        2924
               OH2
                    WAT
                         S1728
                                      57.473
                                                29.684
                                                         48.797
                                                                   1.00
                                                                         33.94
MOTA
        2925
               OH2
                    WAT
                         S1729
                                       0.205
                                                29.580
                                                         11.300
                                                                   1.00
                                                                         28.38
ATOM
        2926
               OH2
                    WAT
                         S1730
                                      28.982
                                                12.144
                                                         36.663
                                                                   1.00
                                                                         22.16
MOTA
        2927
               OH2
                         S1731
                    WAT
                                      -2.247
                                                31.885
                                                         18.386
                                                                   1.00
                                                                         37.56
ATOM
        2928
               OH2
                    WAT
                         S1732
                                      19.593
                                                14.821
27.052
                                                         28.910
                                                                         29.82
                                                                   1.00
                                                                                      S
ATOM
        2929
               OH2
                    WAT
                         S1733
                                       1.174
                                                         34.363
                                                                   1.00
                                                                         22.10
                         S1734
S1735
MOTA
        2930
               OH2
                    WAT
                                      35.909
41.887
                                                         47.248
                                                11.924
                                                                         27.93
                                                                   1.00
                                                                                      S
ATOM
        2931
               OH2
                    WAT
                                                40.436
                                                         52.838
                                                                   1.00
                                                                         28.22
ATOM
        2932
               OH2
                    WAT
                         S1736
                                      26.213
                                                19.454
                                                         10.997
                                                                   1.00
                                                                         22.64
                                                                                      S
MOTA
        2933
               OH2
                    WAT S1737
                                      34.114
                                                42.884
                                                         34.175
                                                                  1.00 28.42
MOTA
        2934
                    WAT $1738
               OH2
                                      22.945
39.089
                                                32.302
                                                         53.065
                                                                   1.00
                                                                         25.85
                                                                                      S
ATOM
        2935
               OH2
                    WAT S1739
                                                15.172
                                                         28.466
                                                                  1.00
                                                                         31.20
        2936
                        S1740
MOTA
               OH2
                    WAT
                                      47.610
                                                43.601
                                                         46.621
                                                                   1.00
                                                                         36.15
                                                                                      S
        2937
MOTA
               OH2
                        S1741
                    WAT
                                      16.327
                                                45.853
                                                         37.179
                                                                   1.00
                                                                        17.39
ATOM
        2938
               OH2
                    WAT
                        S1742
                                                                        29.21
                                      55.363
                                               25.260
                                                         59.367
                                                                   1.00
                                                                                      S
ATOM
        2939
               OH2
                    WAT
                        S1743
                                      30.641
                                               36.731
                                                         14.630
                                                                   1.00
                                                                        26.83
ATOM
        2940
                        $1744
               OH2
                    WAT
                                      10.864
                                               46.250
                                                         10.531
                                                                   1.00
                                                                        23.96
                                                                                      s
                   WAT
                        S1745
S1746
MOTA
        2941
               OH<sub>2</sub>
                                      33.170
                                               48.399
                                                         28.312
                                                                  1.00
                                                                        27.45
MOTA
        2942
               OH2
                                      32.054
                                               14.892
                                                         42.067
                                                                   1.00
                                                                        24.32
                                                                                      s
                   WAT
ATOM
        2943
               OH2
                        S1747
                                      42.724
                                               28.782
                                                         21.018
                                                                  1.00
                                                                        34.32
ATOM
        2944
               OH2
                   WAT
                        S1748
                                      51.123
                                               15.697
                                                         52.194
                                                                        27.97
                                                                   1.00
ATOM
        2945
                                                         56.140
13.736
               OH2
                   WAT
                        S1749
                                      42.354
                                               43.166
                                                                  1.00
                                                                        29.49
ATOM
        2946
               OH2
                   WAT
                        S1750
                                      28.037
                                               37.891
                                                                  1.00
                                                                        33.67
                                                                                      s
        2947
MOTA
               OH2
                   WAT
                        S1751
                                      51.086
                                               26.646
                                                         30.768
                                                                  1.00
                                                                        30.84
        2948
MOTA
               OH2
                   WAT
                        S1752
                                      10.931
                                               38.592
                                                         10.467
                                                                  1.00
                                                                        25.71
        2949
ATOM
               OH2
                   WAT
                        S1753
                                      25.655
                                               29.886
                                                         60.929
                                                                  1.00
                                                                        19.64
                                     17.145
44.748
24.658
        2950
ATOM
               OH2
                   WAT
                        S1754
                                               13.376
                                                         23.383
                                                                  1.00
                                                                        34.23
MOTA
        2951
               OH2
                   WAT
                        S1755
                                               12.372
                                                         45.391
                                                                  1.00
                                                                        18.99
MOTA
        2952
               OH2
                   WAT
                        S1756
                                               10.868
                                                                  1.00
                                                        33.101
                                                                        39.56
                                     10.322
57.341
MOTA
        2953
               OH2
                   WAT
                        S1757
                                               35.265
                                                        39.792
                                                                  1.00
                                                                        31.55
MOTA
        2954
               OH2
                   WAT
                        S1758
                                               22.537
                                                         45.377
                                                                  1.00
                                                                        16.36
                                                                                      S
ATOM
        2955
               OH2
                   WAT
                        S1759
                                      9.420
                                               34.820
                                                        36.963
                                                                  1.00
                                                                        32.92
                                                                                      S
        2956
ATOM
               OH2
                   WAT
                        S1760
                                      32.502
                                               28.596
                                                         14.854
                                                                  1.00
                                                                        21.37
                                                                                      S
MOTA
        2957
               OH<sub>2</sub>
                   WAT
                        S1761
                                     39.205
                                               22.929
                                                        17.441
                                                                  1.00
                                                                        35.60
                                                                                      S
ATOM
        2958
               OH<sub>2</sub>
                   WAT
                        S1762
                                     20.840
                                               52.812
                                                         17.278
                                                                  1.00
                                                                        31.30
                                                                                      S
MOTA
        2959
                   WAT S1763
               OH2
                                     34.711
                                               11.735
                                                        35.138
                                                                  1.00 32.11
                                                                                     S
```

MOTA	2960	OHO	MAT.	S1764	51.666	34.131	47.365	1.00 35.34	s
ATOM	2961	OH2	WAT	S1765	-2.014	36.180	15.830	1.00 28.16	S
ATOM	2962	OH2	WAT	S1766	15.482	48.721	37.060	1.00 29.26	s
ATOM	2963	OH2	WAT	S1767	40.630	14.716	31.062	1.00 40.40	S
ATOM	2964	OH2			23.698	61.256	21.533	1.00 16.86	S
ATOM	2965	OH2							Š
			TAW	S1769	24.781	28.532	54.977	1.00 16.20	3
MOTA	2966	OH2	wat	S1770	26.852	25.257	10.061	1.00 30.41	S
ATOM	2967	OH2	WAT	S1771	43.726	10.405	46.878	1.00 29.13	s
ATOM	2968	OH2	WAT	S1772	25.837	37.362	54.027	1.00 21.97	S
ATOM	2969	OH2							Š
			WAT	S1773	33.373	46.686	32.566	1.00 26.20	5
MOTA	2970	OH2		S1774	27.264	20.817	13.545	1.00 22.02	S
MOTA	2971	OH2	WAT	S1775	47.925	30.806	31.477	1.00 33.49	S
MOTA	2972	OH2	TAW	S1776	8.238	38.202	37.592	1.00 26.28	S
ATOM	2973	OH2		S1777	21.090		25.222	1.00 18.54	Š
						51.641			2
ATOM	2974	OH2		S1778	6.267	38.069	32.873	1.00 22.17	S
ATOM	2975	OH2	\mathbf{WAT}	S1779	23.234	49.347	16.745	1.00 24.08	s
ATOM	2976	OH2	WAT	S1780	22.134	39.856	40.656	1.00 21.00	s
ATOM	2977	OH2	WAT	S1781	20.856	35.405	9.637	1.00 23.13	s
ATOM	2978	OH2							2
				S1782	21.475	53.999	26.047	1.00 27.01	s
ATOM	2979	OH2		S1783	34.915	27.212	15.190	1.00 31.71	s
MOTA	2980	OH2	WAT	S1784	45.211	12.993	42.137	1.00 21.38	S
ATOM	2981	OH2	WAT	S1785	38.126	34.805	40.034	1.00 17.57	s
ATOM	2982	OH2		S1786	30.962	49.798	21.332	1.00 32.31	Š
ATOM									
	2983	OH2	WAT	S1787	33.222	19.319	25.705	1.00 29.22	s
ATOM	2984	OH2		S1788	40.144	19.662	28.253	1.00 33.93	S
MOTA	2985	OH2	WAT	S1789	6.555	28.590	37.281	1.00 28.90	s
ATOM	2986	OH2	WAT	S1790	43.426	43.935	45.155	1.00 34.35	s
ATOM	2987	OH2	WAT	S1791	3.263	33.201	14.705	1.00 33.11	Š
ATOM									2
	2988	OH2		S1792	20.149	16.998	31.047	1.00 26.99	S
ATOM	2989	OH2		S1793	34.123	42.842	21.180	1.00 24.49	S
ATOM	2990	OH2	WAT	S1794	49.929	18.274	53.829	1.00 39.26	S
ATOM	2991	OH2		S1795	14.815	31.617	9.739	1.00 35.94	S
ATOM	2992	OH2		S1796	45.588	41.539	53.753		š
									3
ATOM	2993	OH2	WAT	S1797	33.245	52.433	24.002	1.00 34.85	s
MOTA	2994	OH2	TAW	S1798	43.010	24.276	22.909	1.00 21.38	Š
ATOM	2995	OH2	\mathbf{WAT}	S1799	19.769	14.826	46.718	1.00 30.67	S
MOTA	2996	OH2	TAW	S1800	29.812	17.873	43.458	1.00 28.85	S
ATOM	2997	OH2		S1801	7.028	22.438	24.718	1.00 30.13	s
									5
MOTA	2998	OH2		S1802	7.451	42.723	16.836	1.00 34.86	s
ATOM	2999	OH2	\mathbf{WAT}	S1803	13.062	50.532	16.899	1.00 27.23	S
ATOM	3000	OH2	$\mathbf{T}\mathbf{A}\mathbf{W}$	S1804	31.535	17.528	46.115	1.00 21.48	S
ATOM	3001	OH2	WAT	S1805	1.214	41.199	23.409	1.00 33.03	s
ATOM	3002	OH2	TAW	S1806	12.350	33.958	40.836	1.00 34.82	s
ATOM	3003	OH2		S1807	33.164	41.928	54.755	1.00 33.81	ŝ
									3
ATOM	3004	OH2	WAT	S1808	4.467	50.285	27.482	1.00 36.79	s
MOTA	3005	OH2		S1809	60.702	26.732	42.684	1.00 35.13	
ATOM	3006	OH2	WAT	S1810	22.799	31.560	57.795	1.00 32.80	s
ATOM	3007	OH2		S1811	16.630	35.862	8.507	1.00 29.92	S
ATOM	3008	OH2	WAT	S1812	58.212	35.487	40.540	1.00 33.76	Š
									3
ATOM	3009	OH2		S1813	31.566	17.525	26.426	1.00 39.01	s
ATOM	3010	OH2		S1814	38.884	37.614	20.120	1.00 33.89	S
ATOM	3011	OH2	\mathtt{WAT}	S1815	58.154	24.777	37.822	1.00 35.73	S
ATOM	3012	OH2	WAT	S1816	34.384	14.783	47.649	1.00 37.28	S
ATOM	3013	OH2		S1817	3.439	43.153	36.372	1.00 30.78	Š
	3014						43.290		S
ATOM				S1818	47.394	12.444		1.00 30.32	
MOTA	3015	OH2		S1819	24.644	13.829	44.044	1.00 32.65	S
ATOM	3016	OH2	wat	S1820	35.990	42.985	32.322	1.00 29.66	s
ATOM	3017	OH2		S1821	26.914	40.212	9.947	1.00 33.58	S
ATOM	3018	OH2		S1822	40.296	29.386	23.361	1.00 44.10	Š
									3
MOTA	3019	OH2		S1823	42.915	30.163	27.417	1.00 33.23	5
MOTA	3020	OH2	TAW	S1824	14.322	38.428	8.032	1.00 35.73	S
MOTA	3021	OH2	wat	S1825	33.329	16.000	45.385	1.00 29.78	S
MOTA	3022			S1826	55.683	28.168	38.449	1.00 30.81	S
ATOM	3023	OH2	WAT	S1827	18.514	45.706	9.695	1.00 34.33	ē
									3 6
MOTA	3024	OH2		S1828	19.453	54.788	22.809	1.00 42.02	S
ATOM	3025	OH2		S1829	46.686	27.005	20.816	1.00 31.17	S
ATOM	3026	OH2	WAT	S1830	50.779	32.327	54.666	1.00 44.04	S
ATOM	3027	OH2		S1831	5.243	43.614	40.262	1.00 40.69	S
ATOM	3028	OH2		S1832	45.151	43.041	33.919	1.00 28.47	š
				S1833					ž
ATOM	3029	OH2			26.385	11.949	41.104	1.00 33.70	S
ATOM '	3030			S1834	36.104	26.756	17.653	1.00 32.43	S
ATOM	3031	OH2	WAT	S1835	40.585	7.298	41.894	1.00 32.97	s s
MOTA	3032	OH2		S1836	22.940	54.196	16.985	1.00 39.88	S
MOTA	3033	OH2		S1837	53.968	24.450	37.442	1.00 39.29	S
				S1838					S
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LISTE DE SEQUENCES

- <110> CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE UNIVERSITE HENRI POINCARE DE NANCY
- <120> NOUVELLE PROTEINE DE LIAISON AU PHOSPHATE, COMPOSITIONS PHARMACEUTIQUES LA CONTENANT ET SES UTILISATIONS
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Tyr Ala Glu Asn Gly Thr Val Leu Gln Gly Ser Thr Val Ala Ala Val 325 330 335

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Glu Ala Gly Ala Glu Asp Leu Glu Ile Leu Pro Asn Gly Leu Thr Phe Phe Ser Thr Phe Leu Lys Tyr Pro Gly Ile Lys Ser Phe Asp Pro Ser Lys Pro Gly Lys Ile Leu Leu Met Asp Leu Asn Glu Lys Glu Pro Ala Val Ser Glu Leu Ala Ile Met Gly Asn Thr Leu Asp Met Ser Ser Phe 100 Asn Pro His Gly Ile Ser Thr Phe Ile Asp Glu Asp Asn Thr Val Tyr Leu Leu Val Val Ser His Pro Asp Ser Ser Ser Thr Val Glu Val Phe Lys Phe Gln Glu Glu Glu Arg Ser Leu Leu His Leu Lys Thr Ile Thr His Glu Leu Leu Pro Ser Ile Asn Asp Ile Ala Ala Val Gly Pro Glu Ser Phe Tyr Ala Thr Asn Asp His Tyr Phe Ala Asp Pro Tyr Leu Arg Ser Trp Glu Met Tyr Leu Gly Leu Ser Trp Ser Asn Val Val Tyr Tyr Ser Pro Asp Lys Val Arg Val Val Ala Asp Gly Phe Asp Phe Ala Asn Gly Ile Gly Ile Ser Leu Asp Gly Lys Tyr Val Tyr Ile Ala Glu Leu Leu Ala His Lys Ile His Val Tyr Glu Lys His Ala Asn Trp Thr Leu Thr Pro Leu Lys Val Leu Ser Phe Asp Thr Leu Val Asp Asn Ile Ser Val Asp Pro Val Thr Gly Asp Leu Trp Val Gly Cys His Pro Asn Gly Met Arg Ile Phe Phe Tyr Asp Ser Glu Asn Pro Pro Gly Ser Glu Val Leu Arg Ile Gln Ser Ile Leu Ser Glu Asp Pro Lys Val Thr Val Val Tyr Ala Glu Asn Gly Thr Val Leu Gln Gly Thr Thr Val Ala Ala Val 330 Tyr Lys Gly Lys Leu Leu Ile Gly Thr Val Phe His Arg Ala Leu Cys 345 Cys Tyr Leu

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Phe Ser Thr Gly Leu Lys Tyr Pro Gly Ile Lys Ser Phe Asp Pro Ser 65 70 75 80

Lys Pro Gly Lys Ile Leu Leu Met Asp Leu Asn Lys Lys Glu Pro Ala 85 90 95

Val Ser Glu Leu Glu Ile Ile Gly Asn Thr Leu Asp Ile Ser Ser Phe
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Asn Pro His Gly Ile Ser Thr Phe Thr Asp Glu Asp Asn Thr Val Tyr 115 120 125

Leu Leu Val Val Asn His Pro Asp Ser Ser Ser Thr Val Glu Val Phe 130 135 140

Lys Phe Gln Glu Glu Glu Arg Ser Leu Leu His Leu Lys Thr Ile Thr 145 150 155 160

His Glu Leu Leu Pro Ser Ile Asn Asp Ile Ala Ala Ile Gly Pro Glu 165 170 175

Ser Phe Tyr Ala Thr Asn Asp His Tyr Phe Ala Asp Pro Tyr Leu Arg 180 185 190

Ser Trp Glu Met Tyr Leu Gly Leu Ser Trp Ser Asn Val Val Tyr Tyr 195 200 205

Ser Pro Asp Lys Val Gln Val Val Ala Glu Gly Phe Asp Phe Ala Asn 210 215 220

Gly Ile Gly Ile Ser Leu Asp Gly Lys Tyr Val Tyr Ile Ala Glu Leu 225 230 235 240

Leu Ala His Lys Ile His Val Tyr Glu Lys His Ala Asn Trp Thr Leu 245 250 255

Thr Pro Leu Lys Val Leu Asn Phe Asp Thr Leu Val Asp Asn Ile Ser 260 265 270

Val Asp Pro Val Thr Gly Asp Leu Trp Val Gly Cys His Pro Asn Gly 275 280 285

14

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Leu Arg Ile Gln Asn Ile Leu Ser Glu Asp Pro Lys Ile Thr Val Val 305 310 315 320

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Phe Ser Val Gly Leu Lys Phe Pro Gly Leu His Ser Phe Ala Pro Asp 65 70 75 80

Lys Pro Gly Gly Ile Leu Met Met Asp Leu Asp Glu Arg Pro Pro Ser 85 90 95

Leu Glu Glu Leu Arg Val Ser Trp Gly Phe Asp Leu Ala Ser Phe Asn 100 105 110

Pro His Gly Ile Ser Thr Phe Ile Asp Asp Asp Thr Val Tyr Leu 115 120 125

Phe Val Val Asn His Pro Gln Phe Ser Asn Thr Val Glu Ile Phe Lys 130 135 140

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Glu Leu Leu Pro Ser Val Asn Asp Ile Ile Ala Val Gly Pro Ala His 165 170 175

Phe Tyr Ala Thr Asn Asp His Tyr Phe Ser Asp Pro Phe Leu Lys Tyr 180 185 190

Leu Glu Thr Tyr Leu Asn Leu His Trp Ala Asn Val Val Tyr Tyr Ser 195 200 205 Pro Glu Glu Val Lys Leu Val Ala Glu Gly Phe Asp Ser Ala Asn Gly 210 215 220

Ile Asn Ile Ser Pro Asp Lys Lys Tyr Val Tyr Val Ala Asp Ile Leu 225 230 235 240

Ala His Glu Ile His Val Leu Glu Lys Gln Pro Asn Met Asn Leu Thr 245 250 255

Gln Leu Lys Val Leu Gln Leu Gly Thr Leu Val Asp Asn Leu Ser Ile 260 265 270

Asp Pro Ser Ser Gly Asp Ile Trp Val Gly Cys His Pro Asn Gly Gln 275 280 285

Arg Leu Phe Val Tyr His Pro Asn His Pro Pro Thr Ser Glu Val Leu 290 295 300

Arg Ile Gln Asn Ile Leu Ser Glu Lys Pro Ser Val Thr Thr Val Tyr 305 310 315 320

Ile Asn Asn Gly Ser Val Leu Gln Gly Ser Ser Val Ala Thr Ile Tyr 325 330 335

Asp Arg Lys Leu Leu Val Gly Thr Leu Tyr Gln Lys Ala Leu Tyr Cys 340 345 350

Glu Leu

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Ile Gly Glu Arg Leu Leu Asn Phe Arg Glu Arg Val Ser Thr Thr Arg
20 25 30

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Glu Asn Gly Ser Glu Asp Ile Asp Ile Leu Pro Ser Gly Leu Ala Phe

Ile Ser Thr Gly Leu Lys Tyr Pro Gly Met Pro Ala Phe Ala Pro Asp 65 70 75 80

Lys Pro Gly Arg Ile Phe Leu Met Asp Leu Asn Glu Gln Asn Pro Glu 85 90 . 95

Ala Gln Ala Leu Glu Ile Ser Gly Gly Leu Asp Gln Glu Ser Leu Asn 100 105 110

Pro His Gly Ile Ser Thr Phe Ile Asp Lys Asp Asn Thr Ala Tyr Leu 115 120 125

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Phe 145	Glu	Glu	Gln	Gln	Arg 150	Ser	Leu	Ile	His	Leu 155	Lys	Thr	Leu	Lys	His 160
Glu	Leu	Leu	Lys	Ser 165	Val	Asn	Asp	Ile	Val 170	Val	Leu	Gly	Pro	Glu 175	Gln
Phe	Tyr	Ala	Thr 180	Arg	Asp	His	Tyr	Phe 185	Thr	Ser	Tyr	Phe	Leu 190	Val	Leu
Leu	Glu	Met 195	Ile	Leu	Asp	Pro	His 200	Trp	Thr	Ser	Val	Val 205	Phe	Tyr	Ser
Pro	Lys 210	Glu	Val	Lys	Val	Val 215	Ala	Gln	Gly	Phe	Ser 220	Ser	Ala	Asn	Gly
Ile 225	Thr	Val	Ser	Leu	Asp 230	Gln	Lys	Phe	Val	Tyr 235	Val	Ala	Asp	Val	Thr 240
Ala	Lys	Asn	Ile	His 245	Ile	Met	Lys	Lys	His 250	Asp	Asn	Trp	Asp	Leu 255	Thr
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His	Lys	Arg	Met 340	Leu	Ile	Gly	Thr	Ile 345	Phe	His	Lys	Ala	Leu 350	Tyr	Cys
Asp	Leu														

INTERNATIONAL SEARCH REPORT

** stional Application No **/FR2004/002797

A. CLASSIFICATION OF SUBJECT MATTER IPC 7 C07K14/47

According to International Patent Classification (IPC) or to both national classification and IPC

B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols) IPC 7 C07K

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, Sequence Search, BIOSIS, EMBASE, PAJ, WPI Data

Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US 2003/158115 A1 (LIESKE JOHN C ET AL) 21 August 2003 (2003-08-21) abstract example 6 SEQ ID No 16	1-9
X	DATABASE UNIPROT 'Online! EBI; 10 October 2003 (2003-10-10), XP002275669 Database accession no. P35482 the whole document	1-9
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Further documents are listed in the continuation of box C.	Patent family members are listed in annex.
Special categories of cited documents: 'A' document defining the general state of the art which is not considered to be of particular relevance 'E' earlier document but published on or after the international filing date 'L' document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified) 'O' document referring to an oral disclosure, use, exhibition or other means 'P' document published prior to the international filing date but later than the priority date claimed	 'T' later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention 'X' document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone 'Y' document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art. '8' document member of the same patent family
Date of the actual completion of the international search 23 March 2005	Date of mailing of the international search report 01/04/2005
Name and mailing address of the ISA European Patent Office, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31–70) 340–2040, Tx. 31 651 epo nl, Fax: (+31–70) 340–3016	Authorized officer Keller, Y

INTERNATIONAL SEARCH REPORT

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	Action) DOCUMENTS CONSIDERED TO BE RELEVANT Citation of document with indication, where appropriate, of the relevant passages	Polovant to claim No
	Challen of Goodinent, which indication, which appropriate, of the relevant passages	rielevalii to cialii iyo.
A A	KAWASAKI K. ET AL.: "Mineralized tissue and vertebrate evolution: The secretory calcium—binding phosphoprotein gene cluster" P.N.A.S, vol. 100, no. 7, 1 April 2003 (2003–04–01), pages 4060–4065, XP002275668 the whole document	Relevant to claim No.

Information on patent family members

FR2004/002797

Patent document cited in search report Publication date Patent family member(s) Publication date

US 2003158115 A1 21-08-2003 US 6482934 B1 19-11-2002

RAPPORT DE RECHERCHE INTERNATIONALE

--nde Internationale No '/FR2004/002797

A. CLASSEI	MENT DE	'OB IET	DEIA	DEMANDE
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CTR 7		14/47	,	

Selon la classification internationale des brevets (CIB) ou à la fois selon la classification nationale et la CIB

B. DOMAINES SUR LESQUELS LA RECHERCHE A PORTE

Documentation minimale consultée (système de classification suivi des symboles de classement)

CIB 7 CO7K

Documentation consultée autre que la document à lion minimale dans la mesure où ces documents relèvent des domaines sur lesquels a porté la recherche

Base de données électronique consultée au cours de la recherche internationale (nom de la base de données, et si réalisable, termes de recherche utilisés)

EPO-Internal, Sequence Search, BIOSIS, EMBASE, PAJ, WPI Data

Catégorie °	Identification des documents cités, avec, le cas échéant, l'indication des passages pertinents	no. des revendications visées
X	US 2003/158115 A1 (LIESKE JOHN C ET AL) 21 août 2003 (2003-08-21) abrégé exemple 6 SEQ ID No 16	1-9
X	DATABASE UNIPROT 'Online! EBI; 10 octobre 2003 (2003-10-10), XP002275669 Database accession no. P35482 le document en entier	1-9
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Date à laquelle la recherche internationale a été effectivement achevée	Date d'expédition du présent rapport de recherche internationale
23 mars 2005	01/04/2005
Nom et adresse postale de l'administration chargée de la recherche internationale Office Européen des Brevets, P.B. 5818 Patentlaan 2 NL – 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Fax: (+31-70) 340-3016	Fonctionnaire autorisé Keller, Y

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Catégorie °	identification des documents cités, avec, le cas échéant, l'indication des passages pertinents	no. des revendications visées
-~.cA0110		TIU. GES REVERGICATIONS VISEES
A	KAWASAKI K. ET AL.: "Mineralized tissue	
	and vertebrate evolution: The secretory	
	calcium-binding phosphoprotein gene	
	cluster"	
	P.N.A.S,	
	vol. 100, no. 7,	1
	vol. 100, no. 7, 1 avril 2003 (2003-04-01), pages 4060-4065, XP002275668	
	4060-4065, XP002275668	
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Renselgnements rel ux membres de familles de brevets

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Document brevet cité au rapport de recherche Date de publication Membre(s) de la Date de publication

US 2003158115 A1 21-08-2003 US 6482934 B1 19-11-2002

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